

**INTERNATIONAL UNION OF PURE
AND APPLIED CHEMISTRY**
**UNION INTERNATIONALE DE CHIMIE
PURE ET APPLIQUÉE**

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SECRETARY GENERAL:

Dr. R. Morf, c/o F. Hoffmann-La Roche & Co. Ltd., 4002 Basle (Switzerland)

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LIST OF ABBREVIATIONS

CBN	Commission on Biological Nomenclature
CIG	Comité International de Géophysique
CIOMS	Council for International Organizations of Medical Sciences
COSPAR	Committee on Space Research
ECOSOC	Economic and Social Council of United Nations
FAGS	Federation of Astronomical and Geophysical Services
FAO	Food and Agriculture Organization
IAEA	International Atomic Energy Agency
IAMS	International Association of Microbiological Societies
IASH	International Association of Scientific Hydrology
IAU	International Astronomical Union
IBP	International Biological Programme
IBRO	International Brain Research Organization
ICRO	International Cell Research Organization
ICSU	International Council of Scientific Unions
IGU	International Geographical Union
IGY	International Geophysical Year
IMU	International Mathematical Union
IQSY	International Years of the Quiet Sun
ISO	International Organization for Standardization
ITU	International Telecommunication Union
IUB	International Union of Biochemistry
IUBS	International Union of Biological Sciences
IUCr	International Union of Crystallography
IUCN	International Union for the Conservation of Nature and Natural Resources
IUCRM	Inter-Union Commission on Radio Meteorology
IUGG	International Union of Geodesy and Geophysics
IUGS	International Union of Geological Sciences
IUNS	International Union of Nutritional Sciences
IUPAC	International Union of Pure and Applied Chemistry
IUPAP	International Union of Pure and Applied Physics
IUPS	International Union of Physiological Sciences
IUTAM	International Union of Theoretical and Applied Mechanics
JCAM	Joint Commission on Atomic Masses
JCAR	Joint Commission on Applied Radioactivity
SCAR	Scientific Committee on Antarctic Research
SCOR	Scientific Committee on Oceanic Research
UMC	Upper Mantle Committee
UNESCO	United Nations Educational, Scientific and Cultural Organization
URSI	Union Radio Scientifique Internationale
WDC	World Data Centre
WHO	World Health Organization
WMO	World Meteorological Organization

ADDRESS TO THE XXI CONGRESS

presented by the President, Prof. V. N. Kondratiev, in Prague

I shall not speak here on the importance of the three directions chosen by our Czecho-Slovak colleagues as the main topics of our Congress. These were treated in a clear and precise way by Prof. KLEMM.

A very great number of congresses, conferences and symposia concerned with various fields of science are convened every year all over the world and their contribution to science is very essential. However, IUPAC Congresses are of a still greater importance, as these are sponsored by a Union representing, in fact, all chemistry and giving its name to meetings of highest quality. Every IUPAC Congress, besides the value it has in promoting science and in offering opportunities for best personal scientific contacts, is also a reflection of the IUPAC activities, and its success is that of the IUPAC as well.

I am quite certain that our XXIst Congress will proceed with utmost success, this is my sincerest wish with which I permit myself to end my short tale.

On behalf of IUPAC I would like to express our heartiest greetings to all participants of our Congress. Thank you.

Prof. V. N. KONDRATIEV, President

INTRODUCTION

During the period between 1918–1938, the International Union of Pure and Applied Chemistry organized its conferences each year. Consequently, the activity of IUPAC and its efficient work were *continuously* increasing.

After 1947, transportation by air changed fundamentally the possibilities of international meetings. The number of participants at the conferences increased rapidly, and so did the expenditure for transportation. IUPAC changed over to bi-annual meetings, with the Conferences and Congresses being held only at uneven years. As pointed out in detail in a circular letter to the President and Secretary of all Divisions, Sections and Commissions, the two years interval between IUPAC Conferences (dictated by economical and financial reasons) has the enormous drawback that work is no longer continuous but is generally interrupted by the two years "sleeping period". In the same circular letter, all officers of IUPAC have been urged to overcome this gap, and this problem—by starting work immediately after each Conference, mainly through correspondence.

Before such work can be started, it is essential that the exact composition of all IUPAC units be made known to everyone. The selection and election of Titular Members, Associate Members, and National Representatives must be done with great care. According to the Statutes, National Adhering Bodies must be informed about newly elected members of IUPAC and be given the veto-right.

This is a valuable safe-guard against wrong selections being made on the international level, but the cumbersome procedure involved delays starting of work considerably.

This "Information Bulletin" therefore is published immediately after the XXIVth Conference, giving a tentative picture of the composition of the various Divisions, Sections, and Commissions, with the understanding that the National Adhering Bodies are still given the privilege of making their vetos in case they cannot approve the appointment of IUPAC members to the various working groups. I hope the National Adhering Bodies will understand the necessity of this early and tentative publication. The "Information Bulletin", as its name implies, gives tentative information and has to be considered as a tool for the establishment of the Comptes Rendus XXIV, which, in its final and approved form, will be published at the end of this year.

Another purpose of the "Information Bulletin" No. 30 consists of giving information about the deliberations at the Conference in Prague, and foreshadows the working programme for the next two years. Such information is most valuable for the new members of IUPAC and gives the necessary background for an immediate start in their work.

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To be confirmed 11 November

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PRELIMINARY SURVEY ON THE DELIBERATION AT THE XXIVTH CONFERENCE IN PRAGUE

A full report with all the appropriate minutes will be published, as usual, in the XXIVTH Comptes Rendus. As already pointed out in the preamble, this will take considerable time and therefore this preliminary information is given as an aid-memoir to those colleagues present at Prague and a preliminary information to all those chemists who had not the privilege of attending the Conference and Congress in Prague. Decisions made in Prague can be summarized:

(1) Council ratified promotion from category A 1 to A 2 for the Adhering Organizations of Canada, France and Italy.

(2) The annual dues were unanimously reconfirmed as follows:

Category	D	100 \$
	C	450 \$
	B 1	800 \$
	B 2	1 600 \$
	A 1	2 600 \$
	A 2	5 000 \$
	A 3	10 000 \$
	A 4	25 000 \$

(3) Prof. KONDRATIEV's memorandum, which contained two main proposals, was approved:

- (a) that each Commission of a Division should be represented in the Division Committee itself, and
- (b) that National Bodies should be invited to send representatives to meetings of Commissions.

(4) The Bureau of IUPAC will act as the editorial board.

The chairman of the Commission on the Teaching of Chemistry, R.S. NYHOLM, now Sir RONALD NYHOLM, has been reconfirmed in his office for an additional period of four years. The Commission will meet in the first week-end of January, in Zurich. The working programme of the Commission has been extended considerably. It is hoped that UNESCO will sufficiently recognize the importance of education in the field of the natural sciences and of chemistry, in particular.

(5) Council, with a great majority, decided that IUPAC be given legal status and be incorporated according to the Swiss Law in Zurich, as a non-profit-making scientific society of public interest (Statute 4.3).

(6) Company Associates. Some 60 companies have applied for the newly established membership of Company Associates (decision made by Council in 1965). Accordingly, advanced scientific information on IUPAC activity is given to such Company Associates, which enables them to take a greater interest in IUPAC activity. Also, co-operation of chemical industry, within the framework of IUPAC, in a consulting capacity with United Nations specialized agencies, governmental and non-governmental international organizations, and in particular with the authorities of the European Common Market, is achieved in excellent harmony with this new scheme of IUPAC activity. The names and addresses of those Company Associates who have been accepted by Council, will be listed in detail in the Comptes Rendus

XXIV. Reference is made to the statement made by the President of Applied Chemistry Division, Prof. TRUHAUT, at the meeting in Basle. This statement is reprinted hereafter.

(7) Co-operation with the International Union of Biochemistry (IUB). The shortest way to inform those interested in this very important branch of chemistry is by printing the minutes of the informal discussion between the President of IUB and the officers of IUPAC (see page 31).

(8) Co-operation with the European Common Market (CEE – Communauté Economique Européenne). The coordinating Committee, presided over by Prof. TRUHAUT, in its meeting on Sunday, 3 September, in Prague, explored the possibilities for overcoming the difficulties of finding appropriate staff for drafting data sheets for analytical methods. It was urged that all efforts be made towards fulfilling the contract with the CEE authorities. It is indispensable, that, for the continuation of the co-operation for the coming years, experts and appropriate funds be provided. It is essential that chemists of international standing be consulted whenever chemistry and chemical analysis are involved with legal, social and economical problems, either on a national or international level. Problems of nutrition and health, and the whole human environment, cannot be solved without exact knowledge of chemistry and its impact on life. Criteria of purity, detection of contaminants in air, water and food, cannot be done without the help and advice of chemists. The International Union of Pure and Applied Chemistry is a truly international scientific organization to give advice and help.

(9) A new Division, Division IV on Macromolecular Science, was created. The first constituting meeting will be held on 11–12 November in Brussels.

(10) An independent section on Clinical Chemistry, attached to the IUPAC Bureau, was created.

(11) A task group, to explore the feasibility and the necessity of IUPAC activity in the field of Medicinal Chemistry, was appointed. This task group will report back to the Organic and Applied Chemistry Divisions for a decision at the next Council meeting.

(12) A committee of three experts, convened by TALROSE (USSR), will study the problems of mass-spectroscopy and will report back to the Physical Chemistry Division.

(13) President KONDRATIEV introduced the subject of plasma-chemistry and was given power to make the necessary steps towards making international agreement on symbols, terminology, etc., in this interesting and rapidly expanding field of chemistry.

(14) According to Statute 5405, Council decided that for the next four years English should be the official language for the records.

(15) The invitation by our Australian colleagues to have the XXIInd International Congress in Sydney, from 20–27 August 1969, was confirmed (see page 46).

(16) According to invitation from our Italian chemists, the Council resolved that the XXVth International Conference, associated with a symposium on broad common interests, be held either at the end of June or at the beginning of July 1969, in Italy. It was also reconfirmed that the XXIIIrd Congress and the XXVIth Conference, 1971, be held in Boston and Washington.

(17) Elections. The result of the elections is given with a few exceptions (partly with regard to titular members of Commissions in a tentative way), because the Adhering Organizations might use, in one case or another, the right of a veto (Statute 41303, page 14).

Liaison between IUPAC and industry

In my opinion, IUPAC should be the information centre with which industry would consult, for example, questions of nomenclature, constants, standards of purity, methods of qualitative and quantitative analysis, etc. This is, moreover, the extant situation because every time problems arise in these fields of activity, IUPAC is mentioned as the organization most competent to reply to the query. In this work all the Divisions of IUPAC have a role to play. It is still necessary to create a mechanism which permits a sufficiently rapid answer to be given to the questions posed.

On the other hand, industry can provide IUPAC with a most precious tool of cooperation by furnishing the Union with competent experts. This is of particular importance in the field of Applied Chemistry. The experts of the chemical industry are aware of the practical problems to be solved and could consequently guide the activity of IUPAC towards these problems and contribute in an active manner towards their solution. That is the reason why it is necessary to inject a sufficiently large number of experts from industry into the Sections, Commissions and working groups of the Division of Applied Chemistry, alongside their colleagues from the Universities or government organizations. It would even be desirable, in view of the limitation imposed by the rules of IUPAC upon the number of Titular Members, to appeal for the services of Associate Members belonging to industry and to invite Observers having the same origin.

It is in this direction that the policy of the Division of Applied Chemistry is now aimed; numerous examples of the fecundity of which could be provided. In the long term this policy would have the advantage of interesting industry in the work of IUPAC.

(Statement of the president of the Applied Chemistry Division, Prof. TRUHAUT, at a meeting in Basle, March, 1964.)

Sponsorship

As well as I can remember, this item has been on the Agenda of every IUPAC Meeting. There are many aspects; Scientific meetings, if sponsored by IUPAC, can add to the good name of IUPAC. However, high-quality scientific meetings do not yet need IUPAC's sponsorship. On the other hand, meetings organized in areas where chemistry is not yet sufficiently strong depend on sponsorship, given by great scientists and/or recognized organizations. With a view of protecting its good name, IUPAC must exert some influence on the establishment of scientific programmes of sponsored meetings. Such influence-taking boils down to restrictions put upon the organizers of meetings. Also, the publication policy of IUPAC must be respected.

From what was said before, it is easily understandable that well-established traditional meetings and organizing committees of high recognition in most cases are reluctant to undergo restrictions and therefore refrain from asking for IUPAC's sponsorship. IUPAC's sponsorship in the contrary situation is always asked for from organizers who have not yet sufficient prestige and who are not yet highly recognized on an international level. It is desirable that IUPAC establishes strict rules for giving its sponsorship and sticks to such rules. It is equally essential, and it is statutory that IUPAC stimulates progress and development in chemistry. These two exigencies can hardly be brought in line; that is why the item of sponsorship will always be on our Agenda.

There is still another even more complicated aspect. There is a world-wide reluctance towards attending the international meetings and there are numerous complaints, mainly from employers and scientific bodies, because there are too many meetings. Indeed, since air companies, travel agencies and commercial congress organizers have detected the scientific traveller, there is an increasing inflation in Congresses, Symposia and Colloquia. IUPAC must fight against such proliferation. Success in this cumbersome and not-gratifying task cannot be reached by a passive standby. Close co-operation with Academies, Universities, employers and Chemical Industries might or will be a first step towards remedying this complicated situation. Subventions and travel allowances might be given by Universities, Academies and employers only for IUPAC sponsored meetings. We, in IUPAC, are very far from such a high prestige!

There is finally another aspect which might be the most important of all: The rapidly expanding air traffic, with its high expenditure, provokes an important discrimination to the attendance to international meetings. Well-established and highly recognized scientists easily obtain travel facilities, whereas young people, like students and graduates, are very seldom seen at international congresses. Also, many Academies, learned Societies and even governments give only travel subventions if the applicant reads a paper. The ultimate result of this policy is a drastic limitation of the number of young chemists attending Congresses, etc. The number of papers is increasing and its quality must decrease. Only if the youth gets abundant facilities for attending international meetings might there be a slight hope for fruitful international cooperation in all aspects!

DIVISION DE CHIMIE PHYSIQUE

Définition proposée pour la «mole»

Voici la définition proposée pour la «mole» telle qu'elle figure dans le rapport de la Commission I.1 du Dr WADDINGTON:

“Mole: The mole is an amount of substance of a system which contains as many elementary units as there are carbon atoms in 0.012 kg (exactly) of the pure nuclide ^{12}C . The elementary unit must be specified and may be an atom, a molecule, an ion, an electron, a photon, etc., or a specified group of such entities.”

IUPAC COMMISSION ON TEACHING OF CHEMISTRY

Report to Council of XXIVth Conference

Prague, 29 August–1 September 1967

1. Introduction

Our first report to the IUPAC Conference Council was delivered in Paris in July 1965. On that occasion we outlined our objectives, indicating the subjects to which high priority was to be given. Considerable progress has been made since that time, but the rate at which we are able to proceed is still seriously affected by the need for more financial help. We are grateful to the IUPAC Treasurer and Council for part of our funds and to UNESCO for assistance with specified projects. Help from UNESCO is unfortunately limited to projects in which they are specifically interested; this is understandable in view of their constitution. By overlapping certain activities of UNESCO and IUPAC it is possible to bring together the members of our Commission at periodic intervals to discuss our work. However, it is essential that detailed written reports be available for evaluation by members before coming to the meeting. This involves commissioning people to write these Reports; of course they naturally receive our honorarium and some expenses. So far this sum has been very modest (£50–£100) and in no way compensates for the time and effort involved. Ideally good technical/secretarial help is needed to collect and classify educational data from various countries. Unreliable data is worse than no data; thus on two subjects upon which Reports were commissioned by the British Government recently it was later shown that early *tentative* conclusions were erroneous because of inadequate or erroneous information.

We have also been reluctant up to now, to sponsor large Chemical Education Conferences until adequate information was available for discussion. We feel that far too many educational conferences fail to reach effective conclusions because the delegates discuss *opinions* rather than *established factual data*.

We believe however, that the time has now come when we can usefully sponsor Conferences both National and International on Chemical Education topics and have some specific proposals to put before the Council of the XXIVth IUPAC Conference as discussed below. It must be stressed however that we have no funds at present to hold such Conferences and have had to emphasize this to various interested groups who are keen to obtain our support.

2. Developments since July 1965

Our first report has been published; this dealt with the effect of Examinations upon the Curricula of Chemistry in Schools (the Matthews Report). This has been widely acclaimed as pin-pointing various important problems, but it was necessarily limited in scope to *written* examinations. It is hoped to produce a supplement dealing with Continental Type Oral Examinations, but so far it has not been possible for the person responsible for this to complete the job. We are keen to foster, in due course, a discussion which will bring out the relative advantages and disadvantages of the two systems and ideally provide guidance as to the proportion which seems desirable at various levels of sophistication in the teaching of Chemistry.

The Committee also obtained a draft report on the In-Service Training of Chemistry Teachers and this has been discussed. It was felt that before this was published as a IUPAC Report some supplementation with data from a wider range of countries was necessary. This work has now been completed

and the Report should be available shortly. However, even *before* the Report is published it was considered that a formal recommendation should be made to the Council as a matter of urgency. Recognizing that the *factual* content of Syllabuses is changing today even more rapidly than ever before and that the *approach* to the teaching of chemistry *via* the use of more physical principles (especially thermo-dynamics and energetics generally) frequent and adequate re-training courses for teachers are essential. If adopted it is hoped that wide publicity can be given to the following recommendation as an authoritative statement from the IUPAC Executive to member countries. The resolution is "That in-service training for teachers should be introduced to provide for a minimum of four weeks, preferably three months, re-training every five years for all teachers of chemistry in all countries at the secondary or high school level".

A third Report is at present being prepared for discussion at the end of 1967. This deals with "the extent to which recruitment of students into the study of chemistry at the tertiary level is decreasing in member countries". Data are available to the United Kingdom where the decline is very serious. (Not only has the percentage of students studying Chemistry at the A Level [roughly equivalent to first-year chemistry in the USA, Australia, New Zealand and many Continental Universities] fallen dramatically during the past five years but last year the absolute number of candidates decreased by over 1000.) A similar situation obtains in Mathematics and Physics. One of the effects in the United Kingdom is that whereas there are many good applicants for places in Arts and the Social Sciences there were 1600 *vacant* places in Science and Technology in British universities in October 1966.

We are anxious to obtain reliable data before discussing the reasons for the decline in the United Kingdom but many possible reasons and tentative solutions have already been advanced. It is feared that similar polarisation away from chemistry is occurring in many other member countries of IUPAC. We believe that not only must we encourage more students to obtain degrees in Chemistry but also more Chemistry graduates need to be encouraged to teach Chemistry in schools—where the students are deciding on their future careers. It is hoped to commission a Report on "Methods for the Supply and Recruitment of Chemistry Teachers" in the near future.

3 *Future Activities*

We are also very much concerned with the education and training of technicians. Attention is drawn to the valuable article on "A Basic Curriculum for Chemical Technicians" as outlined in "Chemical and Engineering News" of 22 May 1967. This was produced by the American Chemical Society *ad hoc* Technicians Curriculum Committee. We hope to present a report covering other countries at a later date.

Finally we consider that the retraining of chemists in industry, government service and private practice needs careful consideration. We would welcome the views of Delegates on the desirability of holding an International Conference on the Retraining of Chemists, dealing both with

- retraining of chemistry teachers,
- retraining of chemists in industry, government service and private practice

Such a conference could review the methods at present being adopted to achieve the above and stimulate authorities in member countries both to *allow* and *encourage* chemists to be brought up-to-date.

In conclusion I would like to thank all members of our Commission on the Teaching of Chemistry, especially our secretary Mr D. CHISMAN for their help at all times. Comments on the foregoing from member countries during and after the Prague Meeting will be greatly welcomed.

R.S. NYHOLM, Chairman

PROPOSED IUPAC COMMITTEE ON CONGRESS ORGANIZATION AND PROGRAMMES

Recommendation to the Bureau from the United States Delegation

The Delegation from the United States of America recommends that the Bureau considers the establishment of an IUPAC standing Committee on Congress Organization and Programmes. Our preliminary analysis of the problems that the National Adhering Organization for the United States will face in planning and managing the 1971 Congress of IUPAC makes us believe that such a Committee could be very valuable. In our view, the proposed Committee could assist in several areas:

- (1) From its records, and from the knowledge and experience of the Committee members, it could give important operational advice to the National Committees responsible for individual Congresses.
- (2) It could give assistance in selection of the components of the scientific programmes of the Congresses.
- (3) It could assess the successes and difficulties of each Congress as it occurs and use these observations to recommend appropriate changes in organization or programming for subsequent Congresses.
- (4) It could develop, for potential use by the Bureau, specific recommended procedures for programme development, manuscript review and selection, and other aspects of the best organization of Congresses.

We are persuaded that the continuity and expertise this Committee could provide would be very helpful to all National Committees charged with responsibility for an IUPAC Congress.

IUPAC-IUB COMBINED COMMISSION ON BIOCHEMICAL NOMENCLATURE

THE NOMENCLATURE OF LIPIDS*

Preface

The nomenclature of lipids is the concern both of organic chemists and of biochemists. The systematic names of individual lipids can always be derived by the general rules of organic nomenclature; however, such names are often complex and need to be supplemented by alternative "semi-systematic" names (as has been done, e.g., for steroids and corrinoids). Another problem is that of names for groups of related and homologous compounds (including mixtures); such names are hardly ever needed by the pure organic chemist, but are very necessary in biochemical work.

Several attempts have been made in the past to standardize nomenclature in the lipid field, notably by the United States NAS-NRC Sub-Committee on the Nomenclature of Biochemistry under the Chairmanship of W.E.M. LANDS (Ann Arbor, Michigan) in 1962. At about the same time, proposals were made for names for groups of lipids by a German group (see *Biochem.Z.* 335, 423, 1962).

The Biological Nomenclature Commission of IUPAC and the Commission of Editors of Biochemical Journals of IUB decided, in 1963, to set up an international Sub-Committee on Lipid Nomenclature under the Chairmanship of H. HIRSCHMANN (Cleveland, Ohio); this group discussed and, with the advice of interested colleagues, modified some of the material embodied in the two earlier proposals. The IUPAC-IUB Sub-Committee, which later became responsible to the Combined Commission on Biochemical Nomenclature of IUPAC and IUB (CBN), when this was formed in January 1964, has consisted of the following: H. HIRSCHMANN (Chairman, USA), A. GOTTSCHALK (Australia), F. D. GUNSTONE (UK), M. L. KARNOVSKY (USA), E. KLENK (Germany), W. E. M. LANDS (USA), J. POLONOVSKI (France), L. L. M. VAN DEENEN (Netherlands). Their discussions were carried out largely by correspondence and resulted in draft proposals that were considered by CBN at its meetings in Paris (1965) and in Gothenburg (1966) and by correspondence between the meetings. The present proposals are the product of these events, and are published for the consideration of interested colleagues. It is hoped that discussion will shortly lead to the formulation of Tentative Rules acceptable to chemists in the field of lipids.

CBN is greatly indebted to the members of the Subcommittee on Lipid Nomenclature for their labors. The Introduction, prepared by the Sub-

* A document for discussion sponsored by the IUPAC-IUB Commission on Biochemical Nomenclature, approved by the Commission in April 1967 and published by permission of the International Union of Pure and Applied Chemistry, the International Union of Biochemistry, and the official publishers of the International Union of Pure and Applied Chemistry, Butterworths Scientific Publications.

Comments on these proposals may be sent to any member of CBN: O. HOFFMANN-OSTENHOF (Chairman), W. E. COHN (Secretary), A. E. BRAUNSTEIN, J. S. FRUTON, B. KEIL, W. KLYNE, C. LIÉBECQ, B. MALMSTRÖM, R. SCHWYZER, E. C. SLATER, or corresponding member, N. TAMIYA.

Reprints of these proposals may be obtained from W. E. COHN, Director, NAS-NRC Office of Biochemical Nomenclature, Oak Ridge National Laboratory, Box Y, Oak Ridge, Tenn., 37830, USA.

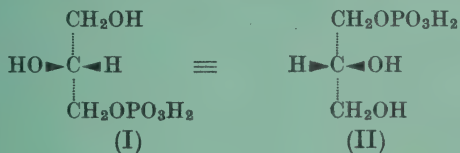
committee, explains the need for a rather novel departure in nomenclature, that of *stereospecific numbering*, which we believe to be worthy of detailed trial and consideration in the special circumstances that obtain in the lipid field.

Introduction

The most complex problem faced by the Subcommittee on the Nomenclature of Lipids concerned the distinguishing of stereoisomers. In the case of glycerol, at least four different systems of designations have been proposed and have been adopted by various authors. All of these proposals possess advantages and disadvantages and none is ideal for all purposes. In view of this situation, it seems desirable to set forth the principal considerations that prompted the selection made by the Subcommittee.

All assignments of configuration in this area rest on the pioneering work of E. BAER and H. O. L. FISCHER and, if priority and widest use were the sole criteria, the system first proposed by these workers (J. Biol. Chem., 128, 475, 1939) would have to be chosen. This system provided that "an α -monoglyceride is to be put in the same category with that glyceraldehyde into which it could be transformed by oxidation without any alteration or removal of substituents" and "since we can without constraint consider the α -glycerophosphoric acids as monoglycerides, their coordination is subject to the same points of discussion". A serious limitation of this nomenclature was stated in the original publication: "An optical classification similar to that which we have suggested for the α -monoglycerides seems to be impossible for the triglycerides."

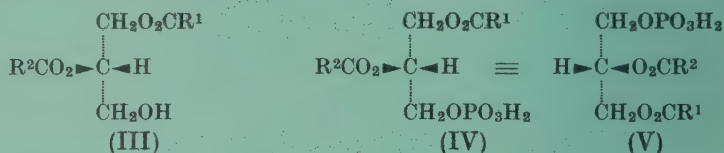
This nomenclature was later extended (E. BAER and D. BUCHNEA, J. Amer. Chem. Soc., 81, 1758, 1959) to compounds that could not be named under the original rule, such as "L- α -(dioleoyl)-cephalin", but as yet no extension has been proposed for the designation of the antipodal forms of, *e.g.*, triacylglycerols or of isotopically labeled glycerols. The system has been criticized by D. M. BROWN, B. F. C. CLARK and R. LETTERS (J. Chem. Soc., 3774, 1961) who stated that "confusion can, and does, arise from whether α refers to the 1- or the 3-position" and by J. BADDILEY, J. G. BUCHANAN and B. CARSS (J. Chem. Soc., 1869, 1957): "The correct name for the naturally occurring L- α -glycerophosphate (I) according to standard rules of nomenclature, is



D-glycerol 1-phosphate (II) (equivalent to L-glycerol 3-phosphate)." A more conventional nomenclature, which also employs D/L prefixes, using numerals as locators and (usually) giving the substituted primary carbinol group the lower number (M. L. KARNOVSKY, G. HAUSER and D. ELWYN, J. Biol. Chem., 226, 881, 1957; A. A. BENSON and B. MARUO, Biochim. Biophys. Acta, 27, 189, 1958) therefore came into use. This system is readily applicable to triacylglycerols, labeled glycerol, etc. Unfortunately, the coexistence of two systems that usually employ antipodal configurational prefixes for the same substance is a potential source of confusion and ambiguity that can be avoided only if the sole outward sign indicating which convention is being followed (the use of Greek letters or numbers as locators, respectively) is always shown and recognized.

This difficulty is avoided if the *R/S* system (R. S. CAHN, C. K. INGOLD and

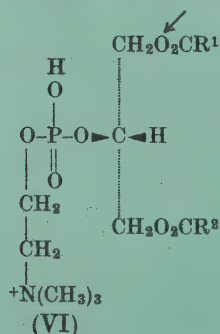
V. PRELOG, *Angew. Chem. Internat. Edit.*, **5**, 385, 1966) is adopted. Its universal character and its freedom from ambiguity have everything to recommend it as the general system and, therefore, the one to be used for information retrieval. However, like the two D/L systems, when applied to glycerol derivatives, it does not bring to the fore important structural and biochemical relationships and therefore does not always provide a convenient terminology for the formulation of significant generalizations. Only a few examples are given. A large part of the chemical and biochemical reactions in the field of glycerol derivatives involves the formation and cleavage of ester and ether linkages. Although these transformations do not affect any of the four bonds that extend from the C-2 of glycerol, the description of these processes under the rules of the *R/S* or D/L system requires frequent changes of the configurational prefixes. For example, the phosphorylation of (*S*)-1,2-diacylglycerol (III) gives an (*R*)-phosphatidic acid (IV). The correspond-



ing transformation under the Baer-Fischer system is

D- α , β -diacylglycerol (III) \rightarrow diacyl-L- α -glycerophosphoric acid (IV). Under the conventional D/L system the precursor (III) is L-1,2-diacylglycerol and the product might be formulated and named as either

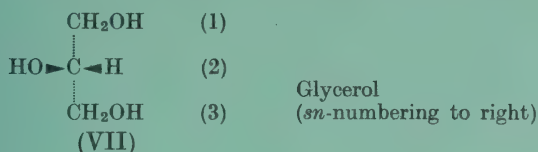
L-1,2-diacylglycerol 3-phosphate (IV) or as D-2,3-diacylglycerol 1-phosphate (V) [III \rightarrow (IV \equiv V)]. If the former is chosen, the formal inversion is avoided, but it would be required in describing the removal of the acyl groups since the product can be properly named only as D-glycerol 1-phosphate (II) [(IV \equiv V) \rightarrow (I \equiv II)]. Furthermore, the enzyme phospholipase A (EC. 3.1.1.4) differentiates between two ester linkages in optically active (and inactive) 1,3-diacylglycerol-2-phosphorylcholines (VI) G. H. DE HAAS



and L. L. M. VAN DEENEN, *Biochim. Biophys. Acta*, **84**, 469, 1964), but this stereospecificity cannot be expressed by the configuration of the substrate in either D/L or *R/S* terms. Still another problem arises if one reports observations demonstrating that the distribution of fatty acids attached to the primary carbinol groups in triacylglycerols is not random. The use of the traditional configurational symbols (D/L or *R/S*) for the description of the asymmetry of such complex mixtures seems quite inappropriate.

These diverse matters present no problem if the stereochemistry of glycerol derivatives is expressed by a fourth system (*stereospecific numbering*,

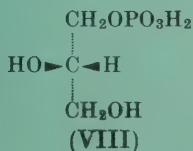
H. HIRSCHMANN, J. Biol. Chem., 235, 2762, 1960), which takes recognition of the fact that the two primary carbinol groups of the parent substance, glycerol, are not identical in their reactions with dissymmetric structures, which include nearly all biochemical processes (A. G. OGSTON, Nature, 162, 963, 1948) and that they therefore should be distinguished in nomenclature. On this basis, the numbers 1 and 3 should not be used interchangeably for the same primary carbinol group. The system proposed for deciding which carbinol group is to receive the lower number is a general one and is based on the priorities of the *R/S* system of CAHN *et al.* Its application to glycerol (VII)



is particularly simple: If the secondary hydroxyl group is shown to the left of C-2 in a Fischer projection, the carbon atom above C-2 is called C-1, the one below C-3; the use of this *stereospecific numbering* is indicated by the prefix "*sn*" before the stem-name of the compound. With such a terminology for distinguishing the two primary carbinol groups of free glycerol, it seemed a logical extension to describe the stereochemistry of derivatives by indicating the carbon atoms that are substituted. This additional step was first taken by R. STJERNHOLM and H. G. WOOD (J. Biol. Chem., 235, 2757, 1960), who spoke of glycerol 3-phosphate. (This would become "*sn*-glycerol 3-phosphate" in the nomenclature proposed here; cf. (I)). Under this system, there can be no formal inversions as long as the four bonds of C-2 remain intact; a given primary carbinol group will always have the same number no matter what the *O*-substituent on this or the other primary carbinol may be. Therefore, identity of configuration is obvious at a glance; e.g., under the *sn* system, the phosphorylation mentioned above is the conversion of a 1,2-diacyl-*sn*-glycerol (III) to a 1,2-diacyl-*sn*-glycerol 3-phosphate (IV).

Similarly, the specificity of the action of phospholipase A can be expressed by stating that it acts on the ester linkage at C-1 (indicated by the arrow) of 2-*sn*-phosphatidylecholine (VI). The non-random distribution of fatty acid residues might conveniently be expressed by such statements as "the 1-position contained most of the saturated fatty acids in the triacyl-*sn*-glycerols of rat liver" (W. E. M. LANDS, R. A. PIERINGER, P. M. SLAKEY and A. ZSCHOCKE, Lipids 1, 444, 1966).

The main disadvantage of the *sn*-system of specifying configurations lies in the fact that it does not express *chirality* in the usual manner by configurational prefixes. This innovation is not altogether without precedent since MAQUENNE in 1900 used numbering in a stereospecific sense to specify the configurations of the inositols. Although the use of *D* and *L* or of *R* and *S* shows more clearly an antipodal relationship, the fact that C-1 and C-3 lie across a plane of symmetry of glycerol should be sufficient to show that *sn*-glycero-1-phosphoric acid (VIII) and *sn*-glycero-3-phosphoric acid (I) are optical antipodes.



PROPOSED RULES

1. Lipids containing glycerol

A. Individual Compounds

1.1 In designating esters, ethers, and other *O*-derivatives of glycerol, rules 10 and 11 of the Rules of Carbohydrate Nomenclature (J.Org.Chem., 28, 281, 1963) are followed. These rules provide that: (1) if the hydrogen atom of an alcoholic hydroxyl group is replaced by another atom or group, the name of the parent compound may be retained as the root of the substituted compound and that, in such names, the prefix (denoting the substituent) is attached directly to the root; (2) an ester may be named by placing after the unchanged name of the parent compound, and separated therefrom by a space, the appropriate numeral (indicating position) and a hyphen, as prefix to the name of the anionic group derived from an acid.

If the substitution is on the carbon atom, the compound is designated by its systematic name and not as a derivative of glycerol. It is permissible, therefore, to omit the symbol "*O*" if the substitution is on the oxygen atoms of glycerol.

Examples: Glycerol tristearate, or tristearoylglycerol or tri-*O*-stearoylglycerol; 1,3-benzylideneglycerol or 1,3-*O*-benzylideneglycerol; glycerol 2-(dihydrogen phosphate) (a permissible alternative to this term is "glycero-2-phosphoric acid")

1.2 In order to designate the stereochemistry of glycerol derivatives, the carbon atoms of glycerol are numbered stereospecifically. The carbon atom that appears on top in that Fischer projection that shows a vertical carbon chain with the secondary hydroxyl group to the left is designated as C-1. To differentiate such numbering from conventional numbering conveying no steric information, the prefix "*sn*" (for stereospecifically numbered) is used. This term is printed in *lower case italics*, even at the beginning of a sentence, and it immediately precedes the term signifying glycerol and is separated from it by a hyphen. The prefix "*rac*-" (for *racemo*) precedes the full name if the product is an equal mixture of both antipodes, and the prefix "*X*-" if the configuration of the compound is either unknown or unspecified.

Examples: *sn*-glycerol 3-(dihydrogen phosphate) or *sn*-glycero-3-phosphoric acid for the stereoisomer previously known as either L- α -glycerophosphoric acid (E.BAER and H.O.L.FISCHER, J. Biol.Chem., 128, 491, 1939) or as D-glycerol 1-phosphate (A.A. BENSON and B.MARUO, Biochim.Biophys.Acta, 27, 189, 1958); *rac*-1-hexadecylglycerol; *X*-glycerol 1,2-dipalmitate 3-stearate

B. Generic Terms

1.3 The term "phosphoglyceride" signifies any derivative of glycerophosphoric acid that contains at least one *O*-acyl, or *O*-alkyl, or *O*-alk-1'-en-1'-yl group attached to the glycerol residue. If the other ester component of a phosphoglyceride is known, it can be stated in a word that precedes the generic term.

Example: Choline phosphoglyceride

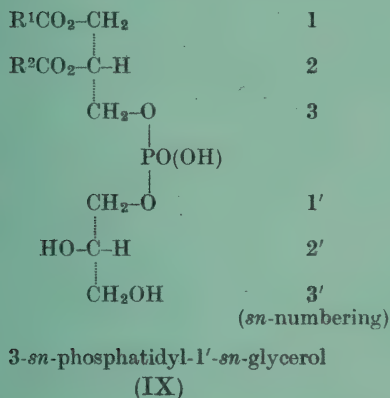
1.4 The term "phosphatidic acid" signifies a derivative of glycerophosphoric acid in which both remaining hydroxyl groups of glycerol are esterified with fatty acids.

1.5 The term "lecithin" is permitted but not recommended to designate a 1,2-diacyl-*sn*-glycero-3-phosphorylcholine. The recommended generic term for such compounds is 3-*sn*-phosphatidylcholine.

1.6 Other generic terms may be coined as needed. These should be patterned after the names of individual compounds (see 1A) and should indicate the type of substituent of glycerol by such prefixes as acyl, alkyl or alkenyl (for alk-1'-en-1'-yl, i.e., R-CH=CH-). If the nature of these substituents cannot be specified, the prefix "radyl" may be used.

Examples for rules 1.4 and 1.6:

phosphatidic ester;
 1-alkenyl-2-acyl-*sn*-glycerophosphoric ester;
O-(diradylglycerophosphoryl)-L-serine;
O-(1-acyl-*sn*-glycero-3-phosphoryl)ethanolamine;
 triacylglycerol;
 diacyl-*sn*-glycero-3-phosphoryl-1'-*sn*-glycerol or
 3-*sn*-phosphatidyl-1'-*sn*-glycerol for structure (IX)



Comment: The terms triacylglycerol, diacylglycerol are preferred for neutral fats, not only for consistency, but mainly because strict interpretation of the traditional (optional) terms triglyceride, diglyceride does not convey the intended meaning.

2. Sphingolipids

A. Individual Compounds

The discovery of many compounds structurally related to sphingosine makes it desirable to develop a semi-systematic nomenclature affording more concise names than the general rules of organic-chemical nomenclature.

2.1 The compound previously known as dihydrosphingosine, 2*D*-amino-öctadecane-1,3*D*-diol or *D-erythro*-2-aminoöctadecane-1,3-diols or (2*S*,3*R*)-2-aminoöctadecane-1,3-diols, is called sphinganine.

2.2 This name may be modified by prefixes to indicate additional substituents or higher or lower homologs. The prefixes to designate homologs should be derived by deleting the terminal "ne" from the systematic names of the hydrocarbons (cf. IUPAC Nomenclature of Organic Chemistry 1957, Rule A-1; also J.Amer.Chem.Soc., 82, 5545, 1960) that have the same number of carbon atoms as the long-chain bases.

2.3 The configuration of additional substituents should be specified by the prefixes "*D*-" or "*L*-" (italic capitals, cf. J. A. MILLS and W. KLYNE, *Progress in Stereochemistry*, 1, 181, 1954) following the number that indicates the position of the substituted carbon atom. The configurations at C-2 and C-3 should be specified in the same manner, but only if they differ from those in sphinganine. In every case, the prefixes *D* or *L* refer to the orientation of the functional groups to the right or left, respectively, of the carbon chain written vertically in a Fischer projection with C-1 on top. If the configuration is unknown, the prefix "*X*-" should be used. In the case of racemic mixtures, the term "*rac*-" should be used as a prefix to the name.

Comment: The semisystematic nomenclature for the long-chain bases is significantly shorter than fully systematic names *only* if the terms chosen imply not only substituents but also their configurations. The configurations usually encountered have identical configurational prefixes only if a *D/L* but not if the *R/S* system is used; e.g., C-3 is *D* and *R* in sphingosine and *D* and *S* in the compound previously known as phytosphingosine. Therefore, the rule that configurations at C-2 and C-3 are to be specified only if they differ from those in sphinganine is unambiguous only if the *D/L* system is used. Whenever it is desired to use the *R/S* system (R. S. CAHN, C. K. INGOLD and V. PRELOG, *Angew. Chem., Int. Edition* 5, 385, 1966), the fully systematic names should be used with specification of configuration at every center (and, when applicable, of the geometry at the double bond).

2.4 Names for partly unsaturated compounds are derived from the names of the corresponding saturated compounds by terminations denoting unsaturation, namely "ene", "diene", "yne", etc. A double bond is presumed to have the *trans* orientation of the carbon chain unless *cis* or unknown geometry is specified by the terms "*cis*-" or "*x*-" preceding the number that indicates the position of the double bond.

Examples for rules 2.1 to 2.4:

4*D*-hydroxysphinganine for phytosphingosine;
4*X*-hydroxy-2*X*, 3*X*-eicosasphinganine for the cerebrin base described by M. PROSTENIK and N. Z. STANAČEV (*Chem. Ber.*, 91, 961, 1958);
4-sphingenine for sphingosine;
cis-4-sphingenine for the geometric isomer of sphingosine;
2*L*-sphinganine for the C-2 epimer of sphinganine

2.5 The trivial name "sphingosine" may be retained. If trivial names other than sphingosine are used, they should be defined in each paper in terms of this nomenclature, or of the general nomenclature of organic chemistry.

B. Generic Terms

Definition:

The term "long-chain base" as used in section 2 refers to sphinganine, its homologs and stereoisomers, and to the hydroxy and unsaturated derivatives of these compounds.

2.6 The following generic terms may be used for the following groups of compounds:

sphingolipid, for any lipid containing a long-chain base;
glycosphingolipid, for any lipid containing a long-chain base and one or more sugars;

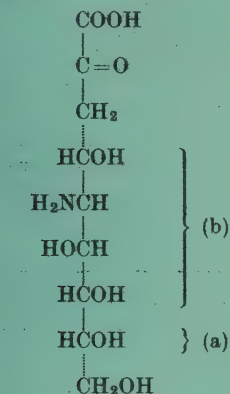
ceramide, for an *N*-acyl long-chain base;
 cerebroside, for a monoglycosylceramide;
 ganglioside, for a glycosphingolipid containing neuraminic acid
 (see Section 3);
 sphingomyelin, for a ceramide 1-phosphorylcholine

2.7 If further structural details can be specified, appropriate prefixes should be used. These prefixes signify substitution and not definition or modification of a component already implied in the root name.

Examples: 1-*O*-D-galactosylceramide, but not galactosecerebroside;
N-acyl-1-*O*-D-galactosyl-4-sphingenine, if the structure of the
 long-chain base can also be specified;
 1-triglycosylceramide;
 oligoglycosylceramide

3. Neuraminic Acid

3.1 The compound 5-amino-3,5-dideoxy-D-glycero-D-galacto-nonulosonic acid is neuraminic acid (X).



Neuraminic acid

[5-Amino-3,5-dideoxy-D-glycero-D-galacto-
 nonulosonic acid] (a) (b)

(X)

3.2 The term "sialic acid" signifies the *N*-acylneuraminic acids and their esters and other derivatives of the alcoholic hydroxyl groups.

3.3 The radicals resulting from the deletion of a hydroxyl group of neuraminic acid or sialic acid are designated as neuraminoyl or sialoyl, respectively, if the hydroxyl is deleted from the carboxyl group, and as neuraminosyl and sialosyl, respectively, if the hydroxyl group is removed from the anomeric carbon atom of the cyclic structure.

4. Other Components of Lipids

4.1 Fatty acids and their radicals should be named according to the IUPAC rules for the Nomenclature of Organic Chemistry, section C-4. Fatty acids should always be numbered with the carboxyl group as C-1.

Comment: Regularities, such as the position of double bonds in some naturally occurring fatty acids, that are not apparent if numbering is done in this manner, can be indicated without violation of this principle of numbering if the position of the double bond is stated in the form ($n-x$) where n indicates the number of carbon atoms in the chain. The positions of the double bonds of linoleic acid, e.g., may be given as ($n-9$) and ($n-6$) but not as $\omega 9$, $\omega 6$.

4.2 Long-chain alcohols and the radicals derived from them should be designated according to systematic nomenclature*, but not by trivial names that are derived from those of fatty acids.

Example: 1-hexadecanol and 1-hexadecyl, but not palmityl alcohol and palmityl.

4.3 Other components of lipids, such as amino acids and sugars, should be named according to the internationally adopted conventions for these groups of compounds.

4.4 All trivial names or abbreviations that are not defined in the rules of sections 1-4 or the other rules cited should be defined in each paper.

5. Other Generic Terms

5.1 The term "phospholipid" may be used for any lipid containing a radical derived from phosphoric acid.

5.2 The term "phosphoinositide" may be used for any lipid containing radicals derived from inositol and phosphoric acid.

5.3 Synonyms for the generic terms defined in these rules should not be used, but other terms may be employed if they apply to different groups of lipids. Such non-official generic terms should be defined in each paper and should be so constructed that prefixes denote substituting groups rather than define components already implied in the root name.

* IUPAC, Nomenclature of Organic Chemistry, Section C, 1965 (Pure and Applied Chem., 11, Nos. 1-2, 1965), Rule C-201 and Section A (J. Amer. Chem. Soc., 82, 5545, 1960), Rule A-1 and others.

ABBREVIATED NOMENCLATURE OF SYNTHETIC POLYPEPTIDES (POLYMERIZED AMINO ACIDS)¹

Tentative rules

The numerous studies on the physical, chemical, and biological properties of synthetic polypeptides have brought with them different ways of describing, in abbreviated form, these products, whose structures are often incompletely known. The use of a variety of nomenclatures complicates the literature; hence, a consistent and clearly defined system for naming such polypeptides is desirable. The proposals set forth here, which represent the consensus of many discussions and suggestions, should aid in systematizing the nomenclature of a wide variety of synthetic polypeptides.

These proposals are based in large part on the abbreviated nomenclature devised by T. J. GILL III [1] and by M. SELA and others (see [2]). They utilize the abbreviations and conventions set forth in Section 2 of *Revised Tentative Rules for Abbreviations and Symbols of Chemical Names of Special Interest in Biological Chemistry* [3] and in *Abbreviated Designation of Amino Acid Derivatives and Peptides* [4], and they add only those terms or conventions needed for the specification of polymers but not encompassed by these schemes. The abbreviations and conventions of the previous Tentative Rules [3, 4] used in this nomenclature system are summarized as follows:

The abbreviations of the amino acid residues and their derivatives or modifications are those indicated in the Tentative Rules [3, 4] or formulated according to the principles set out in them. Hyphens or commas between the symbols for residues or groups of residues mean known or unknown sequence, respectively, and involve only the α -NH₂ and α -COOH groups (the peptide link). [Commas may be omitted when other symbols (e.g., subscripts or superscripts) separate symbols in unknown sequences.] Vertical strokes indicate covalent bonds involving functional groups or the remaining H-atom of the peptide bond, depending upon their placement [4]. L-amino acids and α -peptide links, read from left (NH₂-terminus) to right (COOH-terminus), are assumed unless indicated otherwise [3, 4].

Definitions

1. **Linear polymer:** all amino acids are in an unbranched chain.
2. **Graft polymer:** one or more polymeric segments are linked to the functional groups of a linear chain, thus creating a branch or branches. (Functional groups include ϵ -NH₂, β - or γ -COOH, etc., and the remaining H-atom of an α -peptide link.)
3. **Block polymer:** two or more linear or graft polymeric segments are linked to form a larger polymer.
4. **Polymeric segment:** a polymer that forms a distinct part of a larger polymer (e.g., a block or graft polymer may contain several polymeric segments).

Rules

1. *Polymeric segments* that contain more than one amino acid symbol are enclosed in parentheses or brackets. A superscript outside of the parentheses indicates the number of repeating sequences per 100 residues of polymer, and it is given to the first decimal place.

2. The molar percentage of a single type of amino acid residue within a copolymer, derived from the amino acid analysis and assuming copolymerization, is indicated by a superscript attached to the symbol of the residue. The molar percentages are given in whole numbers and should total 99–101%.

3. *Designation of polymeric segments or linear polymers.* The prefix “poly” or the subscript “*n*” indicates “polymer of”. It is attached to each main chain and is repeated in each polymeric segment within a larger polymer unless there is sufficient indication of size and of structure to make this repetition unnecessary. For example, poly Glu or (Glu)_{*n*} for polyglutamic acid, and (Glu)₁₀ for a decapeptide of glutamic acid.

Comment: “*n*” replaces the “*p*” as originally, but no longer (1967 revision) used in the polymer nomenclature scheme devised by the IUPAC Subcommittee on the Nomenclature of Macromolecules [5]. It is used in designating polynucleotides (see Section 5 of *Abbreviations and Symbols of Chemical Names of Special Interest in Biological Chemistry*, *loc. cit.*), and it is chosen in place of “*p*” in order to avoid confusion with the “*p*” used for a phosphoric acid residue in the latter scheme. The “*n*” may be replaced by a definite number (e.g., 10 above), an average (e.g., 10), or a range (e.g., 8–12), as appropriate.

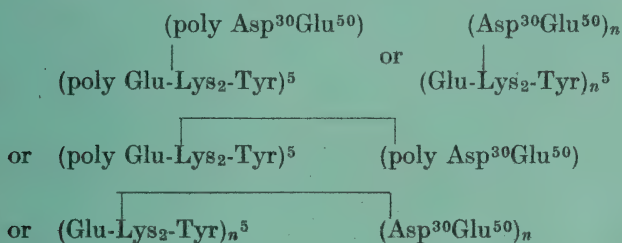
4. *Designation of branches and branch points.* Branches (side chains) connected to the main chain can be designated in one of three ways: by a vertical line joining the main chain and the branch (side chain); by an extended bond joining the appropriate residues with the main chain written first; or by a horizontal double dash (not preferred). The branch points are indicated by the origin and terminus of the vertical line. If the origin is *unknown*, the line originates at the “*p*” in “poly”, if “poly” is used, or at the first parenthesis (bracket), if the subscript “*n*” is used (see Rule 1). If the origin is *known*, the line originates (a) vertically at the initial letter of the appropriate symbol, if functional groups other than α -NH₂ or α -COOH residues are involved; (b) vertically at the position of the appropriate link, if substitution for the remaining H-atom of a peptide link is involved; or (c) horizontally to the left or right of the symbol, respectively, if α -NH₂ or α -COOH groups are involved. The same rules apply to the termination of the line. Thus, the linkage between a side chain functional group and an α -NH₂ or α -COOH group in the main chain is indicated by two perpendicular lines with the vertical line originating in the functional group and the horizontal line in the α -NH₂ or α -COOH group. A number in parentheses lying beside the line indicates the number of such links per 100 residues of polymer, if known.

Comment: A limitation of the double dash as a connecting link lies in its inability to originate or to terminate definitively in a specific residue. Either the arrangement of the symbols must be such that connected ones are adjacent, or the information must be given independently.

Examples

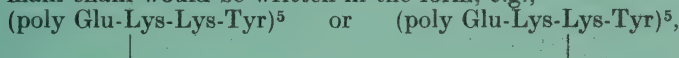
1. Simple homopolymer: poly Ala or (Ala)_{*n*}
2. Linear copolymer, random sequence, composition unknown: poly DLAla,Lys or (DLAla,Lys)_{*n*}
3. Linear copolymer, alternating sequence, composition unknown: poly DLAla-Lys or (DLAla-Lys)_{*n*}
4. Linear sequence of unknown order [composition: 56% Glu, 38% Lys, and 6% Try ($\Sigma = 100\%$)]:
(a) poly Glu⁵⁶Lys³⁸Tyr⁶ or (Glu⁵⁶Lys³⁸Tyr⁶)_{*n*} (all L)

- (b) poly D⁵⁶Glu⁵⁶D³⁸Lys³⁸Tyr⁶ (only Tyr is L)
 (c) poly DL⁵⁶Glu⁵⁶Lys³⁸D⁶Tyr⁶ (Glu is DL, Tyr is D)
5. Block polymer of poly Glu combined through the α -COOH terminus to the α -NH₂ terminus of poly Lys [composition: 56% Glu, 44% Lys ($\Sigma = 100\%$)]:
 poly Glu⁵⁶-poly Lys⁴⁴ or (Glu⁵⁶)_n-(Lys⁴⁴)_n
6. (a) Known, repeating sequence (a polymer of Glu-Lys-Lys-Tyr):
 poly Glu-Lys₂-Tyr or (Glu-Lys₂-Tyr)_n
 (b) Known, repeating sequences within each of two constituent blocks of a linear polymer [composition: 37.5% Glu, 25% Lys, 25% Tyr, 12.5% Ala ($\Sigma = 100\%$)]:
 (poly Glu-Lys)²⁵-(poly Ala-Tyr₂-Glu)^{12.5}
 or (Glu-Lys)_n²⁵-(Ala-Tyr₂-Glu)_n^{12.5}
 [The connection between the polymeric segments shown here is from the α -COOH of Lys to the α -NH₂ of Ala. Origin or termination in any other residue or functional group can be shown by rearranging the order of residues and by the orientation of the connecting line at its origin and terminus (see Examples 7, 8, 9).]
 (c) Known, repeating sequence in the main chain connected by the ϵ -NH₂ of a lysine (which of the two is not known) to an unknown point in an unknown sequence in the side chain [composition: 30% Asp, 55% Glu, 10% Lys, 5% Tyr ($\Sigma = 100\%$)]:



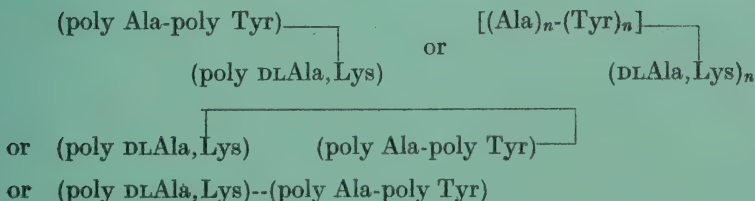
(Note: The double hyphen system is not applicable here.)

If the lysine residue connected to the side chain were known, the main chain would be written in the form, e.g.,



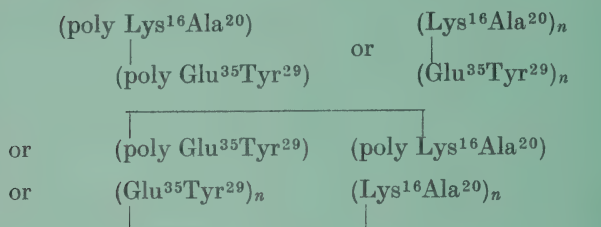
as appropriate.

7. Graft polymer with the main chain of DL-alanine and L-lysine connected through the ϵ -NH₂ group of lysine to the α -COOH group of L-tyrosine in the side chain, which consists of a block polymer of L-tyrosine and L-alanine (no analytical data for the main chain):

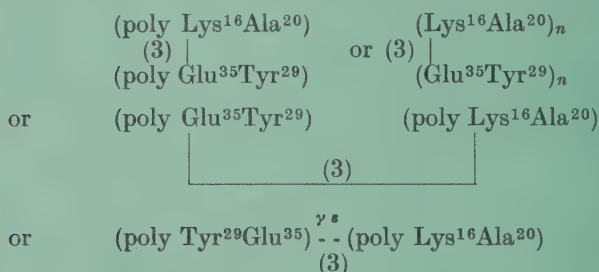


(Note: The points of attachment of Lys and Tyr cannot be specified in the last example.)

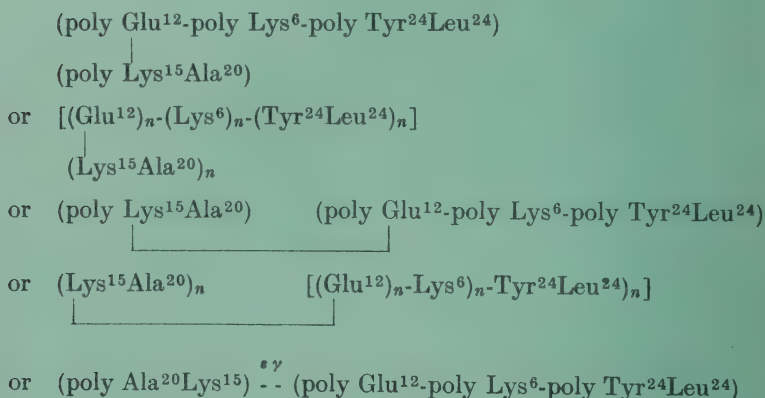
8. Graft polymer with an unknown sequence in the main chain and in the side chain [composition: 16% Lys, 20% Ala, 35% Glu, 29% Tyr ($\Sigma = 100\%$)]:
- (a) Number and position of the points of attachment in the main chain unknown, but terminating in the lysine residues of the side chain:



- (b) Same, but attachments are 3 in number and connect the $\epsilon\text{-NH}_2$ groups of the lysine residues in the side chain and the $\gamma\text{-COOH}$ groups of the glutamic acid residues in the main chain:



9. Graft polymer with a block polymer and an unknown sequence in the side chain (upper) attached to an unknown sequence in the main chain (lower); the points of attachment are between the $\gamma\text{-COOH}$ groups of glutamic acid in the side chain and the $\epsilon\text{-NH}_2$ groups of lysine in the main chain [composition: Glu 12%, Lys 21%, Tyr 24%, Leu 24%, Ala 20% ($\Sigma = 101\%$)]:



References

1. Biopolymers 2, 283 (1964). [See also J.Biol.Chem. 240, 3227 (1965); Biochim.Biophys.Acta 124, 374 (1966).]
2. Advances in Immunology 5, 30 (1966).
3. J.Biol.Chem. 241, 527 (1966); Biochemistry 5, 1445 (1966); Biochem.J. 101, 1 (1966); Virology 29, 480 (1966); Arch.Biochem.Biophys. 115, 1 (1966); Europ.J.Biochem. 1, 259 (1967); Zeit.Physiol.Chem. 348, 245 (1967).
4. J.Biol.Chem. 241, 2491 (1966); Biochemistry 5, 2485 (1966); Biochim.Biophys.Acta 121, 1 (1966); Biochem.J. 102, 23 (1967); Arch.Biochem.Biophys. 121, 1 (1967); Europ.J.Biochem. 1, 375 (1967); Z.Physiol.Chem. 348, 256 (1967); Bull.Soc.Chim.Biol. 49, 121 (1967).
5. J.PolymerScience 8, 257 (1952). [1967 Revision in press.]

Footnote

¹ Document of the IUPAC-IUB Commission on Biochemical Nomenclature, approved by CBN, IUPAC and IUB in September 1967 and published by permission of the International Union of Pure and Applied Chemistry, the International Union of Biochemistry, and the official publishers of IUPAC, Messrs Butterworths Scientific Publications.

Comments on these Tentative Rules may be sent to any member of CBN: O. HOFFMANN-OSTENHOF (Chairman), W. E. COHN (Secretary), A. E. BRAUNSTEIN, J. S. FRUTON, B. KEIL, W. KLYNE, C. LIÉBECQ, B. G. MALMSTRÖM, R. SCHWYZER, C. E. SLATER; or corresponding member, N. TAMIYA.

Reprints of these Tentative Rules may be obtained from WALDO E. COHN, Director, NAS-NRC Office of Biochemical Nomenclature, Biology Division, Oak Ridge National Laboratory, Box Y, Oak Ridge, 37830, Tenn., USA.

COOPERATION IUB/IUPAC

Minutes of the informal discussion held in London on 28 April 1967

Were present: President IUB Prof. S. OCHOA, Prof. W. KLEMM and Dr R. MORF.

(1) Arising from the Minutes of the 58th Executive Committee Meeting of IUPAC and in particular from the proposals to Bureau and Council, it was suggested that

- (a) Division of Biochemistry be discontinued
- (b) IUB/IUPAC Nomenclature Commission be continued and attached to Division III
- (c) Clinical Chemistry be made a *Section*
- (d) IUB invite IUPAC to delegate an ex-officio Member of IUPAC to sit on the Bureau of IUB
- (e) IUPAC shall invite IUB to name an ex-officio Bureau Member to sit on the corresponding body of IUPAC
- (f) It was tentatively suggested that, initially, Prof. KLYNE could be designated as the IUPAC ex-officio Bureau Member (subject to approval by Council)
- (g) The time when such arrangements should start would have to be decided at the IUPAC Meeting in Prague and the IUB Meeting in Tokyo, assuming it to be acceptable to both parties

(2) These measures are intended to provide a satisfactory atmosphere for fruitful and close cooperation between the two Unions:

- (a) As a first step in that direction a joint IUB/IUPAC-Ciba Symposium on Stereochemistry be held in 1968 (see letter 5169/RM/sg of 4 April 1967)
- (b) That the two Unions should act concertedly in education and in influencing Editors of Biochemical journals with a view to ironing out and coordinating the pattern of publishing scientific results
- (c) That the two Unions coordinate their efforts in effecting cooperation between the abstracting services in chemistry and biological abstracts

DETAILED INFORMATION REGARDING FORTHCOMING MEETINGS

MODERN CHEMISTRY IN INDUSTRY

Eastbourne, 11-14 March 1968

Designed to promote an increasing flow of school leavers into science and of science graduates into industry. The aim of the conference is to demonstrate the economic and social contributions of an industry based on high scientific attainment and to explore current misconceptions that are believed to exist regarding the respective roles of academic and industrial research

President: The Lord TODD, F.R.S.

Vice-Presidents: Sir SYDNEY BARRATT, J.P. BERKIN, C.B.E., The Hon. Sir MAURICE BRIDGEMAN, K.B.E., Sir PAUL CHAMBERS, K.B.E., C.B., C.I.E., The Lord COLE OF BLACKFRIARS, Sir RONALD CUMMING, T.D., The Lord FLECK, K.B.E., F.R.S., The Lord HILL OF LUTON, The Lord NETHERTHORPE, K.B.E., LL.D., Sir HUGH TETT

Policy Committee: N.A. ILIFF (Chairman), G.F. ASHFORD, O.B.E., Sir RONALD HOLROYD, F.R.S., J.C.H. McENTEE, Prof. H.W. THOMPSON, C.B.E., F.R.S.

Chairman of the Conference Committee: J.D. ROSE

Chairman of the Programme Committee: Dr F.N. WOODWARD, C.B.E.

Honorary Treasurer: Dr J.S. GOURLAY

Honorary Secretary: Lt. Col. F.J. GRIFFIN, O.B.E.

The background of the Conference

In 1964 the President of IUPAC, Lord TODD, set up an international committee to examine ways in which the International Union of Pure and Applied Chemistry could be of greater service to the chemical industry.

One recommendation made was to hold conferences under IUPAC auspices but organized by industry, and devoted largely to scientific research carried out in industrial organizations and designed to demonstrate the extent to which social and economic benefits arising from chemical activities in recent years have been dependent on such work.

The offer of the British National Committee for Chemistry to organize the first of such conferences in the United Kingdom was accepted, and the need for more accurate understanding of the place and standing of science in industry has steadily increased and become more widely recognized.

The Conference on "Modern Chemistry in Industry" is designed to be complementary to other activities aimed to increase the flow of school leavers into science, to rectify some misconceptions about scientific work in industry, and to improve industry's scientific reputation.

It will describe and illustrate the volume and quantity of scientific research carried out by industrial organizations and, while in no way denigrating the valuable work of academic research, it will aim to remove the apparently deep-seated impression that the work of industrial scientists is limited in any way to developing basic discoveries made in the academic world.

The Conference is open to all who wish to participate and will include a proper cross section of professors, readers, lecturers, demonstrators and postgraduate workers in universities, and senior science masters from secondary, grammar and public schools.

It is anticipated that attendance may be in the order of 1500-2000 and arrangements have been made for lecture accommodation in the Congress Theatre and Winter Garden, Devonshire Park, Eastbourne, and for hotel accommodation through Thos. Cook & Son Ltd.

The programme will open on the afternoon of Monday, 11 March, and cover the whole of 12 and 13 March, and will conclude after the morning session on Thursday, 14 March.

The Conference fee is 10 guineas and will include the right of attendance at all sessions of the Conference, a copy of the Summaries of Papers to be read, and a copy of the Proceedings to be published later with all the papers and discussions.

Further details of the Conference and hotel accommodation arrangements, together with a registration card, will be sent to those who complete the enclosed form.

Opening Plenary Session: Modern chemistry in industry

Lord SHERFIELD (ICFC)

Principal T.L.COTTRELL (Stirling University): Interaction between industrial and academic science

Dr M.E.SPAGHT (Shell): Industry, school and university relationships in Europe and the United States

Lord BEECHING (ICI): How British industry sees higher education

Second Plenary Session: The involvement of science in industry

Dr F.N.WOODWARD (Arthur D.Little): Choosing research projects

Dr J.W.BARRETT (Monsanto): Conducting research, hardware and people

Mr M.A.E.HODGSON (ICI): Exploiting research

Specialist Session, Stream 1: Raw materials, energy and human needs

Dr T.M.SUGDEN (Shell): Energy, fuel technology and chemistry

Modern science of petroleum

Mr E.V.WHITEHEAD and Dr H.POWELL (BP): Modern contribution to the study of petroleum constitution

Mr E.S.SELLERS (Humphreys and Glasgow Ltd.): Meeting the requirements of a changing product pattern

Dr J.WOOLCOCK (Humphreys and Glasgow Ltd.): The choice of petroleum products as raw materials for chemical processes

Food production

Dr P. W. REYNOLDS (ICI): Fertilizers

Dr R. A. E. GALLEY (Shell): The protection of crops and stored products

Mr A. CHAMPAGNAT (BP): The biosynthesis of proteins from petroleum

Mr M. J. CAHALAN (Rio Tinto Zinc Corp.): Modern science of winning minerals and metals

Mr C. HOBBS (J. Laing & Son Ltd.): Some applications of chemistry to the construction industry

Dr J. G. COLLINGWOOD (Unilever): Oils and fats

Specialist Session, Stream 2: Invention, design and operation of chemical processes

First-stage petroleum chemistry

Mr G. P. ARMSTRONG (BP): Phenol from cumene process

Dr D. G. JONES (ICI): Importance of basic chemistry on a large-scale process

Dr FRANK B. MARCOTTE (Celanese Research Co., USA): Oxidation of aliphatic hydrocarbons

Dr R. LANDAU (Halcon): Oxidation of aromatic hydrocarbons

Oxygen-assisted processes

Prof. F. R. BRADBURY (Stirling University): The development of the paraquat process

Dr. G. C. FETTIS (ICI): Production of vinyl chloride by the oxychlorination of ethylene

Recent advances in homogeneous catalysis

Prof. G. WILKE (Max-Planck-Institut für Kohlenforschung, Mülheim): Transition-metal catalyzed organic reactions

Dr J. W. CORNFORTH (Shell): New developments in catalysis

Dr G. A. GAMLEN (ICI): The coalescence of modern inorganic and organic chemistry

New frontiers in the design and control of processing plant

Mr D. T. SHORE (AVP): The influence of biochemistry on the engineering design and control of new food processes

Mr R. FOWLER (Power Gas): Trends in the nitrogen fixation industry

Specialist Session, Stream 3: The products of the chemical industry

Polymeric products

Dr R. M. LODGE (ICI): Oriented polymers

Dr W. COOPER (Dunlop): Non-oriented polymers

Prof. C. E. BAWN (Liverpool University): Polymers with special properties — Materials science

Biologically active chemicals

- Dr A. H. COOK (Nutfield): The diversity of yeast chemistry
Dr F. HARTLEY (School of Pharmacy, London University): Steroids and hormone products or therapeutic agents
Dr MILES WEATHERALL (Wellcome Foundation): The discovery of new drugs
Dr J. G. MORLEY (Rolls-Royce): Inorganic materials
Dr C. V. STEAD (ICI): Recent advances in dyestuffs research
Dr R. Price (ICI): Coordination chemistry in dyestuffs and pigments

Final Plenary Session: Can scientists find satisfaction in industry?

- Mr G. F. ASHFORD (BP): As seen through the eyes of an industrialist
Prof. R. V. JONES (Aberdeen University): As seen through the eyes of an academic
Dr D. DAVIES (ICI): The inventive polymath
Prof. MICHAEL M. SWAN (Edinburgh University)

IVTH INTERNATIONAL CONGRESS ON CATALYSIS

Moscow, 23-29 June 1968

Sponsored by the Academy of Sciences of the USSR

Organizing Committee—Executive: *President*: Prof. A. A. BALANDIN, Member of the Academy of Sciences of the USSR. — *Vice-Presidents*: Prof. G. K. BORESKOV, Member of the Academy of Sciences of the USSR, Prof. A. M. RUBINSTEIN, Prof. KH. M. MINACHEV, Prof. B. A. KAZANSKII, Member of the Academy of Sciences of the USSR, Prof. S. Z. ROGINSKII, Corresponding Member of the Academy of Sciences of the USSR, Prof. V. B. KAZANSKII. — *Secretary*: Dr B. D. POLKOVNIKOV. — *Members*: Dr G. G. CHAKHMAKHCHEV, Dr V. S. FEDOROV, Dr I. N. KISELEV, Prof. N. K. KOCHETKOV, Dr S. G. KORNEEV, Dr L. A. KOSTANDOV, Prof. O. V. KRYLOV, Dr E. S. LIKHTENSTEIN, Prof. I. F. LUTSENKO, Prof. B. L. MOLDAVSKII, Prof. A. F. PLATE, Prof. V. A. ROITER, Dr M. M. SAKHAROV, Dr V. S. SMIRNOV, Prof. D. V. SOKOLSKII, Prof. M. I. TEMKIN, Prof. K. V. TOPCHIEVA, Prof. V. A. VINOGRADOV, Prof. TH. TH. WOLKENSTEIN.

The opening of the IVth International Congress on Catalysis will take place on 23 June 1968. The scientific sessions will begin Monday morning, 24 June, and will end in the first half of Saturday, 29 June.

The Moscow Symposia will take place from 1-4 July and the Novosibirsk Symposium will take place from 5-7 July.

The programme of the Congress includes:

- A. 6 lectures
- B. Reports and their discussion

A detailed schedule of the work of the Congress will be available to the participants before its opening.

All those who have sent in an application for participation in the Congress will receive a third circular containing complete information about the work of the Congress.

Registration Forms

Would-be participants of the Congress and Symposia are requested to fill in the enclosed registration forms, each in two copies, and to send them as soon as possible, but not later than 10 January 1968, to the Organizing Committee of the Congress.

Membership Fees

The membership fees for a participant of the Congress (giving the right to take part in both Moscow Symposia) are 30 roubles (US \$33) and for an associate (only members of the family), 10 roubles (US \$11).

The membership fees for participation of a member of the Congress in the Novosibirsk Symposium are 10 roubles and 4 roubles (US \$4.5) for an associate.

All membership fees must be paid not later than 10 January 1968.

The membership fees are payable in US dollars or their equivalent in the currencies of the following countries: Australia, Belgium, Canada, Denmark, England, France, German Federal Republic, Italy, Japan, Netherlands, Norway, Sweden, Switzerland.

The money should be sent to the account of the Organizing Committee at the Bank of Foreign Trade of the USSR: Account No. 0652222 with the Vneshtorgbank of the USSR, address: Neglinnaya, 12, Moscow, USSR.

The fees are not subject to refund.

Scope of the Congress

The IVth International Congress on Catalysis will be devoted to the problem of the "Principles of the Prediction of Catalytic Action". This includes experimental and theoretical investigations into the relations between catalytic activity and the chemical composition, structure and electronic properties of catalysts, that allow predictions of catalytic action to be made.

Papers will be accepted dealing with heterogeneous catalysis or with phenomena common to both heterogeneous and homogeneous catalysis. Both simple and complex heterogeneous catalytic reactions may be discussed.

The main stress will be on the prediction of catalytic activity and selectivity based on studies of reaction mechanisms and of the mode of action and properties of catalysts.

No papers will be considered that are of a purely kinetic or purely adsorption character or those dealing with the structure and physical properties of catalysts without regards to the mechanism of their action. Neither will papers be accepted that relate the catalytic activity to the texture of the catalysts, that are devoted to heat or mass transfer, that are concerned only with homogeneous gaseous or with biological catalysis or that are of a purely phenomenological nature.

In view of the short duration of the Congress and the fact that Symposia will be held on a number of related subjects, the Organizing Committee reserves the right to accept only such papers that are strictly within the scope of the Congress.

Besides reports on original work it is intended to hold 6 lectures of a more general nature on the following subjects:

- (1) Catalysis on metals
- (2) Homogeneous and heterogeneous acid-base catalysis
- (3) Thermochemical correlations in catalysis
- (4) The application of crystal field theory to heterogeneous catalysis
- (5) The stereochemistry of catalysis
- (6) Non-classical two-dimensional surface compounds and their role in catalysis

The Reports and Synopses

It is planned to publish the proceedings of the Congress, including the lectures, papers and discussions in the first half of 1969.

Preprints of the papers accepted for discussion at the Congress will be sent to all participants before its beginning.

Submission of papers is open only to those taking part in the Congress. When a paper is written by more than one author, at least one of the authors must be a participant of the Congress.

Authors will be given 5 min in which to make their reports and 15 min will be allotted to discussion after each report.

Synopses typewritten in English or Russian should be sent to the Organizing Committee in 3 copies not later than 15 July 1967. The synopses should not exceed 500 words and should contain the title of the report, the name(s) of the author(s), the name of the organization(s) to which the author(s) is (are) affiliated and the respective city and country. This should be followed by a concise and clearly formulated statement of the objectives of the report, its main premises, basic results and conclusions. The synopses will not be published.

The typescript of the report should not exceed 30000 printer's signs (5000 words), including tables, figures and references. Each figure counts for 1500 printer's signs; each line of a table, for 150 signs.

Papers will be accepted only if they do not exceed the above-designated size and provided they contain previously unpublished data that fall within the scope of the Congress.

Typescripts of the reports made according to the instructions given below should be sent in 3 copies to the Secretary of the Organizing Committee not later than 15 September 1967. Russian authors and such foreign authors who are in a position to do so should send 3 copies, each, of their papers in English and Russian.

Final selection of the papers will be made by the Organizing Committee from the typescripts it will have received.

Preparation of the manuscripts. On the top of the first page both in the English and Russian versions there should be written: "The IVth International Congress on Catalysis, Moscow, 1968. Preprint."

The title of the paper should be followed by the initials and name of the author(s), the name of the organization(s), the city and country.

This is followed by an abstract of the paper, not exceeding 1200 printer's signs (200 words).

After the abstract comes the text of the paper, itself, which should contain an introduction, experimental part and discussion, preferably in the order mentioned. References in the text are consecutively numbered and the list of references is given at the end of the paper in the following order: initials and name of author(s), the name of the periodical (in standard abbreviation), its volume, year (in parentheses) and page.

Mathematical and chemical formulas and equations should either be typed completely or else neatly filled in with India ink, but there should be no mixing of typed and written characters. Tables are to be given in the text of the typescript and not on separate sheets. They should be numbered in consecutive order and their headings should be as brief as possible.

Drawings. Line drawings (diagrams, nomograms, graphs) should be made in India ink on Whatman paper or on white tracing paper, or else as photographs on dull-surface white paper. The prints should not be larger than 13 cm \times 18 cm. All lettering should be done in India ink, very clearly and of sufficient size as to be legible when diminished by $\frac{2}{3}$. Pictures should be

of the same size as line drawings (not larger than 13 cm × 18 cm) and should be made on dull-surface white paper.

The figures should be numbered consecutively.

The legends to the figures are typed on a separate sheet of paper.

Attention! Instructions for the Typist

In typing the manuscript, please, adhere strictly to the following requirements:

(1) The manuscript must be typed on *white paper 21 cm × 30 cm*, on one side.

(2) All the sheets should have margins of 20 mm at the top and bottom and of 25 mm to the right and left, so that the typed surface is 16 cm × 26 cm.

(3) The abstract is typed at 1.5 intervals and the main text at 2 intervals between lines.

(4) The title of the paper and the headings of its principal parts are typed in capitals. The titles should be positioned at the same distance from the right- and left-hand sides of the sheet.

(5) Subheadings to other (not principal divisions) of the paper are given in low-case letters and begin directly from the margin.

(6) Sentences beginning a new paragraph are indented by 5 spaces.

(7) The letters should be clear and the sheets should have a uniform appearance.

(8) Legends to the figures should be typed on a separate sheet with a distance of 2 intervals between lines and a distance of 4 intervals between consecutive legends.

(9) No corrections should be inserted between lines. In case it is necessary to correct a few misprints, the corrected text should be pasted onto the erroneous text exactly in line with the rest of the typing so as not to stand out in any way.

Slides. Slides should be 24 mm × 36 mm in size and should be mounted in a frame of 5 cm × 5 cm; slides can be also 9 cm × 12 cm in size with the figure in a horizontal position. All slides are made by the author. The auditorium of the Congress will be equipped only for showing diapositive slides, no episcopes being planned.

Languages of the Congress. The official languages of the Congress will be Russian and English. Provisions will be made for translation during the meetings of the reports and discussion from Russian into English. The lectures will be synchronously translated into English, French, German and Russian.

Symposia

It is planned to hold 3 post-Congress Symposia that are listed below. The typescripts of synopses and reports for the Symposia should strictly comply with the requirements given. Synopses should be sent to the Organizing Committee not later than 15 December 1967, and the reports themselves should be sent not later than 15 December 1967.

I. Mechanism and Kinetics of Complex Catalytic Reactions

Moscow, 1-3 July 1968

President of the Organizing Committee of the Symposium: Prof. S. Z. ROGINSKII, Institute of Chemical Physics, USSR Academy of Sciences, Moscow B-334, Vorob'evskoe Shosse, 2b.

The program of the Symposium consists of 2 parts:

(1) General problems concerning the theory of complex catalytic processes and specific methods for investigating the mechanisms of each of their stages.

(2) The selectivity and conjugation catalytic reactions.

(a) Selective reinforcement of one of several possible parallel reactions and the selective formation of products of a given chemical and steric structure.

(b) Evident and hidden conjugation of both similar and differing types of reactions with special stress on the conjugation of oxidation-reduction reactions.

Reports will be favored that deal with new reactions and mechanisms, that advance new concepts or describe new methods of investigation. Reports will be accepted that include data on both heterogeneous and homogeneous catalysis together with their comparison.

No reports will be accepted that are of a purely synthetic or phenomenological nature, that are purely kinetic, without considering the stage-by-stage mechanism, or that are of a purely applied character or deal with particularities in catalytic polymerization, or homogeneous, or biological catalysis without any generalization. Reports are also not acceptable that have been previously published as such or in the form of articles.

It is planned to have 26 papers read at the 6 meetings of the Symposium and of these 4 will be lecture reports. The reports will be made partly by invitation, partly by selection from synopses that will have been sent to the Organizing Committee.

Authors will be given 5 min to make their report. Lecture reports will be allotted 30 min.

II. Electronic Phenomena in Chemisorption and Catalysis on Semiconductors

Moscow, 2-4 July 1968

President of the Organizing Committee of the Symposium: Prof. TH. WOLKENSTEIN, Institute of Physical Chemistry, USSR Academy of Sciences, Moscow B-71, Leninskii Prospekt, 31.

The programme of this Symposium consists of 3 parts:

(1) Various forms of chemisorption on semiconductors; the electronic mechanism of chemisorption and of the catalytic acts.

(2) Relation between the electronic parameters of a semiconductor (electroconductivity, work functions, etc.) and its chemisorptive and catalytic properties.

(3) The effect of irradiation on the chemisorptive and catalytic properties of semiconductors (including photoadsorptive and photocatalytic effects).

Altogether 18 reports will be given during the 6 meetings of the Symposium. The authors will be invited by the Organizing Committee. Each report will contain a review of the present-day status of the problem and also of the original work of the author and his collaborators. The report will be

allotted 30 min and 30 min for discussion; each participant in the discussion will be allowed 5 min.

The reports will be read in Russian, English, French and German. No translations will be made. Discussion will be carried out in any one of the above languages.

Detailed synopses of the reports (2-3 typed pages), will be preliminarily distributed among the participants of the Symposium.

III. The Porous Structure of Catalysts and the Role of Transport Processes in Heterogeneous Catalysis

Novosibirsk, 5-7 July 1968

President of the Organizing Committee of the Symposium: Prof. G. K. BORESKOV, Institute for Catalysis, Siberian Branch of the USSR Academy of Sciences, Novosibirsk, 90.

The programme of the Symposium consists of 2 parts:

(1) Effect of transport processes and of the porous structure of catalysts on the kinetics and direction of catalytic reactions.

(2) Experimental methods of determining the porous structure and mass transport coefficients in the catalyst grain.

Reports will be favored that deal with regularities in the above processes.

There will be 24 reports made during the 5 meetings of the Symposium. The reports accepted will be allotted 5 min for reading, followed by their discussion. The reports will be preliminarily published in English and Russian and will be sent to the participants of the Symposium.

Accommodation

Since June and July is the busiest time for tourism in the Soviet Union, in order to avoid difficulties with hotel reservation and services, the Organizing Committee requests the members of the Congress to make arrangements for their travel to the Soviet Union through the Intourist (USSR Travel Agency).

Class "Luxe"—US \$35 a day per person. This involves the cost of a *single* room with bath, 3 meals a day (menu à la carte), porter and car on arrival and departure, 2-hour excursion in a car with a guide-interpreter, bus from hotel to the seat of the Congress and back. With a *double* room the price will be \$25 a day per person, 1 car and 1 guide-interpreter for 2 persons.

Category A—\$19 a day per person. This involves the cost of a *single* room with bath in first-class hotels, 3 meals a day (first-class menu), porter and car or bus on arrival and departure, bus from hotel to the seat of the Congress and back, 2 group excursions in a bus with a guide-interpreter. With a *double* room the price will be \$16 a day per person.

Category B—\$13 a day per person. This involves the cost of a *double* room without bath in tourist-class hotels, 3 meals a day (tourist-class menu), porter and car or bus on arrival and departure, bus from hotel to the seat of the Congress and back, 2 group excursions in a bus with a guide-interpreter.

Additional information will be given concerning the possibility of accommodating the younger members of the Congress at reduced rates in student dormitories.

Excursions and post-Congress Tours

For participants of the Congress there will be organized visits to Scientific Institutes and visits to museums, historical places and places of interest both in Moscow and in other parts of the Soviet Union.

A detailed schedule of all the nontechnical arrangements of the Congress will be given to the participants during registration.

After the Congress the following scientific tours will be available to participants and their associates through Intourist:

Tour No.1: Moscow-Leningrad-Moscow (1st class)

(4 tour days) 5-9 July 1968—\$93.00

Tour No.2: Moscow-Kiev-Moscow (1st class)

(3 tour days) 5-8 July 1968—\$82.00

Tour No.3: Moscow-Tbilisi-Moscow

(4 tour days) 5-9 July 1968—\$135.00

Tour No.4: Moscow-Novosibirsk-Moscow (1st class)

(5 tour days) 5-10 July 1968—\$234.00

Tour No.4 is open only to participants of the Symposium on the Porous Structure of Catalysts and the Role of Transport Processes in Heterogeneous Catalysis.

The prices indicated cover first-class service including hotel accommodations and transport expenses.

Ladies' Programme. A special programme will be arranged for the ladies, which will include the visiting of museums, art galleries and places of interest in Moscow.

Banquet. A banquet is planned by the Organizing Committee to mark the end of the Congress. The Committee kindly requests those wishing to take part to fill in the attached reservation form and send it together with the registration forms to the Organizing Committee. The price is 10 roubles per person. Payment will be only in roubles and is to be made during registration at the Congress.

Travel Formalities

The travel formalities, including visas, should be arranged solely through tourist agencies. The tour orders should be bought from the foreign Intourist agency contractors.

All applications for tours should be submitted before the deadline of 20 May 1968.

The Intourist will be unable to be of any help to those who did not make hotel reservations in advance and did not buy the tour orders from foreign Intourist agency contractors.

Applications may be submitted only after paying the registration fee.

The Organizing Committee would be very grateful if you would be so kind as to inform all those who might be interested and who have by some oversight failed to receive Circulars No.1 and 2 of the contents of these circulars and in case they manifest further interest to recommend them to write to the Secretary of the Organizing Committee for Circular No.2, simultaneously enclosing 5 typewritten slips of their address.

Correspondence

Please address all correspondence concerning the VIth International Congress on Catalysis to Dr B. D. POLKOVNIKOV, Secretary, VIth International Congress on Catalysis, Moscow, B-334, Leninskii Prosp., 47, Institute of Organic Chemistry, Academy of Sciences of the USSR.

2ND INTERNATIONAL SYMPOSIUM "PHARMACEUTICAL CHEMISTRY"

Münster/Westf. 22-26 July 1968

Sponsored by the Division of Organic Chemistry and the Division of Applied Chemistry of IUPAC

This Symposium will be held 22-26 July 1968 at the Westfälische Wilhelms-Universität Münster/Westf. (Germany).

Topics of the Symposium

New developments in the following fields of drug research:

- Nonsteroid antiinflammatory drugs
- Analgetically acting drugs
- Drugs acting on the blood circulation and the heart
- Chemotherapy of parasitic infections
- Metabolism of drugs

Registration of Papers; Symposium Languages

Participants may present own papers related to these topics with an approximate length of 15 min of speech. They are asked to register not later than 1 April 1968 including an abstract of their contribution. Papers may be read in German, English or French. Service for translation will not be available. In addition main lectures on these topics by distinguished scientists are in preparation. These lectures will be published in "Pure and Applied Chemistry", the official journal of IUPAC. They will also be issued as a specially bound reprint on which a discount of 20% will be allowed on all orders received before the end of the meeting.

Ladies' Programme and Excursions

A ladies programme is planned. Excursions will be arranged for 26 July 1968.

Provisional Applications

Those interested in this Symposium are requested to return the enclosed postcard to the Secretary as soon as possible and not later than 31 January 1968. A preliminary programme and forms for registration will be mailed to them.

Executive Committee

K.E.SCHULTE (Chairman), F.WEYGAND (President, Division of Organic Chemistry), R.TRUHAUT (President, Division of Applied Chemistry), E.SCHRAUFSTÄTTER, W.MEYER ZU RECKENDORF.

Address for Correspondence

The Secretary, 2nd IUPAC Symposium "Pharmaceutical Chemistry", Hittorfstrasse 58-62, 44 Münster/Westf. (Federal Republic of Germany).

XITH INTERNATIONAL CONFERENCE ON COORDINATION CHEMISTRY

*Haifa, 8-12 September 1968,
and Jerusalem, 16-18 September 1968*

The Conference Headquarters will be at the Technion--Israel Institute of Technology, Technion City, Haifa. Scientific Sessions will be held at the Technion in Haifa and at the Hebrew University in Jerusalem.

Scope and Sessions

The Organizing Committee of XIth International Conference on Coordination Chemistry wishes to emphasize a few selected areas of the ever-widening field of Coordination Chemistry. It is therefore proposed to organize several symposia on selected topics, with a main lecture of 45 min followed by several shorter papers. Each symposium session will be concluded with a 60-min general discussion. No parallel sessions will be held during the symposia.

The regular sessions will be grouped into three or four sections. For each paper 25 min will be available including the time for discussion.

The final selection of topics will be made after receipt of completed form A from the intending participants.

Scientific Contributions

All contributions and attendance will be by invitation only. Those wishing to be invited to present a paper should complete all particulars on both the enclosed forms A and B and return them to the Chairman of XIth International Conference on Coordination Chemistry before 15 November 1967.

ANALYTICAL CONFERENCE

Warsaw (Poland), 10-15 September 1968

This Conference will be organized by the Commission of Analytical Chemistry of the Polish Academy of Sciences, under the auspices of International Union of Pure and Applied Chemistry. The scientific programme will be devoted to the following main four branches of analytical chemistry:

- (1) Basic problems as new reagents, new reactions, ionic equilibria, accuracy and precision, etc.
- (2) Analytical methods in inorganic industry
- (3) Analytical methods in organic industry
- (4) Technique of analytical chemistry, e.g. new apparatus, automation, standards, sampling

The intention of the Organizing Committee is to group the scientific papers on the basis of the kind of analyzed material and not on the basis of applied method.

The summaries of papers, which may be presented in English, French, German or Russian, should be submitted to the Conference Secretary not later than 15 January 1968. The time provided for each scientific communication should not exceed 15 min (including discussion). The plenary lectures will be held by invited speakers. During the Conference several scientific and sight-seeing excursions will be provided.

Registration fees amounts US \$20 and 10 for active participants and accompanying members, respectively.

All correspondence should be addressed to Dr ADAM HULANICKI, Secretary of the Organizing Committee, ul. Pasteura 1, Warszawa 22 (Poland).

1968 TRIPARTITE CHEMICAL ENGINEERING CONFERENCE

The Institution of Chemical Engineers is to hold a meeting in North America. This will be a joint meeting with The Canadian Society for Chemical Engineering, which will act as host for the Conference, and the American Institute of Chemical Engineers. The meeting will be held in the Queen Elizabeth Hotel, Montreal, from 22-25 September 1968. Mr C.S. WINDEBANK, Vice-President of The Institution of Chemical Engineers, is Technical Programme Organizer for the UK.

IUPAC-SPONSORED SYMPOSIUM ON CHEMICAL CONTROL OF THE HUMAN ENVIRONMENT

Johannesburg (South Africa), July 1969

It is planned to hold this in *the third week of July 1969*. Since some of those attending the Symposium may wish to go on to the Conference and Congress in Melbourne in August 1969, on the same round trip ticket, consideration is being given to arrangement of tours to other centres of scientific interest in South Africa after the Symposium.

The subject of the Symposium is to be interpreted broadly as dealing with all chemical topics relating to control of environment. Thus, it is not confined to the use of chemicals for control, but includes all chemical and biochemical problems arising from the use of such chemicals, and also the isolation, analysis and identification of chemical substances which are injurious and which therefore should be controlled.

Apart from original papers from both South African and other authors, the opportunity will be taken to present a number of review papers on South African work, where this covers conditions which are outside the experience of most workers in other countries.

Owing to the broad nature of the symposium, a large number of papers is expected so that, to remain within the confines of a single week, at least three sessions will be held concurrently, and speakers will be asked to present summaries only. The medium will be English.

For convenience, the Symposium will be divided into five sections, each of which will be introduced by at least one plenary lecture by a leading scientist in the particular field.

In the following, those aspects which will receive particular attention in each section are outlined, and the names of the corresponding plenary lecturers are given.

1 Control of Air Pollution

will deal with methods for measuring pollution and with methods for reducing pollution to a minimum.

The plenary lecturer will be Prof. Dr WOLFGANG TESKE, who is head of a group of Farbwerke Hoechst AG, Frankfurt (West Germany), which has carried out much research on control of industrial gaseous emissions.

2 *Control of Water Supplies*

will deal with chemical methods of treatment for water supplies and for re-use of effluents.

The plenary lecturer will be Prof. K. J. IVES, of the Department of Civil and Municipal Engineering, University College, London.

3 *Control of Agricultural Pests*

will deal with insecticides, herbicides and chemical lures such as sex attractants in the broadest possible sense, namely, utilization, control of residues, metabolism, etc.

There are two plenary lecturers, namely, Prof. F. A. GUNTHER, Citrus Experimental Station, University of California, who is an authority on analysis of pesticide residues; and Prof. A. S. CRAFTS, Department of Botany, University of California, whose studies have lain in the field of herbicide metabolism.

4 *Control of Health*

The use of chemotherapeutic drugs for human health has been excluded from the symposium since its implications are too vast to be covered in the limited time available. This section is planned therefore to cover two specific subsections.

- (i) Chemical methods for the control of disease-bearing vectors, particularly those of importance to human health
- (ii) Use of antibiotics in agriculture both to combat disease and to facilitate production

It is expected to have a plenary speaker for each of these topics.

5 *Control of Toxic Substances*

can be regarded as a further subsection of 4, as it is concerned with substances injurious to health, both human and animal. It embraces the many harmful substances which can occur in foodstuffs for human consumption; but, in South Africa, a great deal of work has been done on veterinary aspects, due to an abundance of poisonous plants and, in more recent years, to toxins of fungal origin.

The plenary speaker is Dr L. A. GOLDBLATT of the Southern Utilization Research and Development Division, of the US Agricultural Research Service, who is an authority on the field of mycotoxins.

XXIIND INTERNATIONAL CONGRESS OF PURE AND APPLIED CHEMISTRY

and

XIITH INTERNATIONAL CONFERENCE ON COORDINATION CHEMISTRY

Sydney (Australia), 20-27 August 1969

A combined meeting, comprising the XXIInd International Congress of Pure and Applied Chemistry and the XIIth International Conference on Coordination Chemistry, will be held in Sydney, Australia, 20-27 August 1969.

It is expected that the scientific programme of the meeting will be presented under the following main headings:

IUPAC

Physical Chemistry

Theoretical chemistry and molecular spectroscopy—Intermolecular forces—High pressure chemistry—Kinetics—The solid/liquid interface—Polymers and polymerization kinetics

Inorganic Chemistry

Non-metals—Non-transition metals—Interfacial processes in mineral extraction—On-stream analysis in the mineral industry—Solid-state chemistry

ICCC

The nature of the metal-ligand bond—Biological aspects of coordination chemistry—Mechanisms of substitution and electron transfer reactions—Investigation of molecular dissymmetry—Complex equilibria in solution—Reactivity of ligands and catalysis by coordination compounds—Structure and reactivity of organometallic compounds

An International Symposium on Electron and Nuclear Magnetic Resonance will be held in Melbourne, under the auspices of the Australian Academy of Science, shortly before the Sydney meeting.

Congress Languages

Papers may be presented in any language, but the Organizing Committee hopes that speakers will use a language that is widely understood, preferably English.

Correspondence

All correspondence concerning both the XXIIInd International Congress of Pure and Applied Chemistry and the XIIth International Conference on Coordination Chemistry should be addressed to:

The Chairman, Organizing Committee

XXIIInd International Congress of Pure and Applied Chemistry

Box 2249U, GPO

Melbourne (Australia)

or to the Secretary General, CH-4002 Basle (Switzerland)

CALENDAR

1968

March 11-14	Symposium on Modern Chemistry in Industry	Eastbourne (UK)
March 14-16	Symposium on Standards for High Pressure Research	Gaithersburg, Maryland (USA)
April 1-5	Joint Annual Meetings	Dublin (Ireland)
May 13-17	International Symposium on the Recovery of Pulp and Paper Chemicals	Helsinki (Finland)
June 17-21	Symposium on the Structure and Chemistry of Solid Surfaces	Berkeley, California (USA)
June 23-29	IVth International Congress on Catalysis	Moscow (USSR)

July	IIInd International Symposium on the Chemistry of Organic Silicon Compounds	Bordeaux (France)
July 8-11	Symposium on Nuclear Magnetic Resonance	São Paulo (Brazil)
July 8-13	Vth International Symposium on the Chemistry of Natural Products	London (UK)
August	VIth International Symposium on the Reactivity of Solids	Schenectady, New York (USA)
September 4-6	International Conference on Electrophotography (Dr W. LEWIS HYDE, Institute of Optics, University of Rochester, Rochester, NY, USA)	Rochester (USA)
September 8-12 (Haifa) 16-18 (Jerusalem)	XIth International Conference on Coordination Chemistry	Haifa and Jerusalem (Israel)
September 3-6	IIIrd International Symposium on Fermentation	New Brunswick (USA)
September 10-13	Analytical Chemistry Symposium	Warsaw (Poland)
September	Symposium Valence Tautomerism	Karlsruhe (Germany)
1969		
4th week in April	Symposium on Natural Products	Mexico
June or July	XXVth International Conference of Pure and Applied Chemistry including a Symposium	Italy
1st week in July	Symposium on Chemical Control of Human Environment	Johannesburg/Pretoria (South Africa)
July 14-18	IVth International Congress on Pharmacology	Basle (Switzerland)
August 20-27	XXIIInd International Congress of Pure and Applied Chemistry and XIIth International Conference on Coordination Chemistry	Sydney (Australia)
To be decided	Symposium on Nonaqueous Electrochemistry	To be decided
September 7-11	VIth International Symposium on Microchemistry	Graz (Austria)
September 8-13	VIIIth International Congress on Clinical Chemistry	Geneva (Switzerland)
1969 or 1970	International Symposium on Analytical Chemistry	Birmingham (UK)
1970		
	Symposium on the Chemistry on Natural Products organized by the Academy of Science of the USSR	
	Symposium on Carbohydrates Chemistry sponsored by the Division of Organic Chemistry	

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**INTERNATIONAL UNION OF PURE
AND APPLIED CHEMISTRY
UNION INTERNATIONALE DE CHIMIE
PURE ET APPLIQUÉE**

**INFORMATION BULLETIN
NUMBER 31**

MARCH 1968

SECRETARY GENERAL:
Dr. R. Morf, c/o F. Hoffmann-La Roche & Co. Ltd., 4002 Basle (Switzerland)

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INTRODUCTION

Towards the end of the year 1967, when drafting and compiling the Comptes Rendus of the XXIVth Conference, it was extremely difficult to know exactly the composition of the various Divisions, Sections and Commissions. Also, it was not possible to check exactly the addresses of all members of the various units.

Information Bulletin No.31, therefore, will give you additional and up-to-date information about changes in the composition of various Sections and Commissions which have been constituted only recently.

The International Association of National Chemical Societies, which was founded at the end of the XIXth century and which is the forerunner of IUPAC, was indeed a true federation of the various national chemical societies. The first gathering of Presidents of chemical societies was therefore held in the framework of the forerunner of IUPAC.

The American Chemical Society's President, CHARLES OVERBERGER, on 29 and 30 November 1967, followed this excellent example by inviting the heads of nine other chemical societies to Washington.

In various countries, national chemical societies are still strongly tied to IUPAC. The IUPAC representation there is identical with the officers of the national chemical society.

However, in many other countries, national chemical societies have not much influence on the IUPAC's activities.

It has to be pointed out here, as a very favourable evidence and, to some extent as a nouveauté, the fact that at the inaugural meeting of the new Macromolecular Division held in Brussels there were present, among the 10 members of the Division Committee:

the active President of the American Chemical Society, the President-elect of the Chemical Society of London and the President-elect of the American Chemical Society who, on January 1968, has taken the presidency of this largest scientific society of the world.

At a very recent meeting in Zürich of IUPAC's Committee on the Teaching of Chemistry, which is composed of 8 members, there were present

the active President of the Société chimique de France, the President-elect of the Chemical Society of London and one of the past Presidents of the American Chemical Society.

We sincerely hope that these facts are not only a lively demonstration of IUPAC's prestige and of a close cooperation with all the National Chemical Societies within IUPAC but will also mark an important progress in our cooperation.

Finally, the Information Bulletin No.31 gives up-to-date information with regard to the activity program of 1968.

INTRODUCTION

Vers la fin de l'année 1967, dans la compilation des Comptes Rendus de la XXIV^e Conférence, il a été très difficile de connaître exactement la composition des différentes divisions, sections et commissions ainsi que les adresses précises des membres.

Le Bulletin d'information n° 31, en conséquence, a pour but de donner des informations additionnelles aux Comptes Rendus.

Vous trouverez donc une liste complète des sections et commissions qui ont été constituées seulement bien après la conférence de Prague (voir pages 5-12).

L'Association internationale des sociétés chimiques, qui fut créée à la fin du XIX^e siècle et qui a précédé l'IUPAC, formait vraiment une fédération des sociétés chimiques nationales.

Dans plusieurs pays cette idée s'applique encore à l'IUPAC tandis que dans ceux les plus importants du point de vue de la chimie, les sociétés chimiques nationales n'ont pas eu beaucoup d'influence sur l'activité de l'IUPAC.

Il est à relever à présent, à la fois comme une innovation et un signe extrêmement favorable, le fait qu'à la réunion inaugurale de la Division Macromoléculaire tenue à Bruxelles, parmi les 10 membres du Comité de Division, l'on comptait le président actif de l'American Chemical Society, le futur président de la Chemical Society de Londres et le « President-elect » de l'American Chemical Society qui, depuis le 1^{er} janvier 1968, occupe le poste de Président de cette Organisation. A Zurich, à la réunion toute récente du Comité pour l'Enseignement de la Chimie, sur les huit membres composant ce Comité, l'on compte le président actif de la Société Chimique de France, le futur président de la Chemical Society de Londres et l'un des anciens présidents de l'American Chemical Society.

Nous espérons que ces faits ne sont pas seulement une démonstration importante du prestige de l'IUPAC, mais qu'ils sont aussi la marque d'un progrès véritable de coopération.

Finalement, le Bulletin d'information n° 31 indiquera les dernières informations relatives au programme d'activité pour 1968.

COMPOSITION OF DIVISION COMMITTEES, NATIONAL REPRESENTATIVES

Memo by V. N. KONDRATIEV, President, a basic document for discussion by Bureau and Council

I came in closer contact with IUPAC activities in 1961, and since then I have been a member of the Bureau and the Executive Committee. The activities of certain Divisions and Commissions of IUPAC became considerably wider during the past six years, particularly so with respect to the needs of the chemical industry.

The problems arisen in this connection seem to require a somewhat more clear-cut organization of certain IUPAC departments, and the present IUPAC structure is not always adequate to it. Indeed, the IUPAC Commissions and Sections are its main working bodies. The first thing evident is that there is some inconsistency in the memberships of Commissions and of the Divisions Committees heading these Commissions. If the aim of a Committee is to direct, to coordinate and control the work of Commissions, at least one representative of every Commission should be a member of the respective Division Committee. However, the Committee of the Inorganic Chemistry Division, for example, consisting of 11 persons, has only one Commission representative, that from the Commission on High Temperatures and Refractories (II.3). Only two Commission representatives, both from the Chemical Plant Taxonomy Commission (III.2), enter into the Committee of the Organic Chemistry Division consisting of 10 persons. The Committee of the Analytical Chemistry Division (10 persons) involves 7 Commissions and has only three Commission representatives, those from Commissions on Spectrochemical and Other Optical Procedures (V.4), on Electroanalytical Chemistry (V.5), and on Analytical Radiochemistry and Nuclear Materials (V.7). The Committees of the Physical Chemistry and Applied Chemistry Divisions are composed on a more appropriate basis and either presidents or members from all Commissions (with one exception in both cases) enter into these Committees. This makes obviously easier the functioning of Division Committees with respect to their Commissions.

While members of the Division Committees representing one or another Commission are responsible for the contact of the latter with the Division, the functions of other Committee members are not always clear. The principle of fair geographical distribution as motive for inviting representatives of various countries into a Division Committee is warranted when the given Committee member ensures contacts between IUPAC and its National Committee. However, as one person may fulfill this task with respect to problems of his competence only, and cannot represent the whole scope of the multiple Division activities, it becomes evident that one representative of a country cannot ensure all the necessary contacts between the Division and the National Committee of his country. On the other hand, an increase in the number of titular members would be impossible and inexpedient.

A solution to this problem seems to be suggested by the long-term practice of the Applied Chemistry Division. Certain Sections of this Division [that on Oils and Fats (VI.3), on Plastics and High Polymers (VI.7), and on Organic Coatings (VI.8)] have a great number of National Representatives, 77 in all*. If this practice were adopted in all Divisions and Commissions

* It would be of interest to hear from Prof. TRUHAUT about his experience in the work with National Representatives.

and appropriate persons were selected, the contacts between IUPAC and National Committees would be better ensured. I attempt at present to establish such contacts between the National Committee of Soviet Chemists and IUPAC. We have asked certain members of our Committee, and also certain other specialists to study the activities of various IUPAC Commissions and then to establish personal contacts with the chairmen or secretaries of the Commissions.

To begin with I have asked all chairmen of Commissions and Sections, on behalf of the National Committee, to send me a brief report on the present activities and on the future programme. I have received this information from all of them and I thank them most sincerely.

In connection with the above I would make two proposals aimed at ordering and, I believe, at improving the IUPAC structure, namely:

(1) To make the membership of Division Committees more adequate to their tasks with respect to the directions of Commission activities, co-ordination and control. Every member of the Committee would be responsible for certain functions connected with one or another side of the IUPAC activities. This would pertain to associated members as well.

(2) Ensure maximum interaction between IUPAC Divisions, Commissions and Sections and the National Committees in order that the activities of the latter be maximally consistent with the requirements of science and chemical industry in various countries. The contacts between IUPAC and the National Committees might seemingly be ensured by the body of national representatives in every department of IUPAC.

It will be emphasized that in case these proposals are accepted the number of titular members would diminish by some 20 persons.

I understand that these proposals are not always consistent with the long-term traditions of IUPAC, and cannot be accepted without careful discussion, which would require a certain time. I trust that two years would be amply sufficient, so that the necessary reconstruction might have been completed towards the end of my presidency.

signed: V.N.KONDRATIEV

IV

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IUPAC COMMITTEE ON THE TEACHING OF CHEMISTRY

IN-SERVICE TRAINING OF CHEMISTRY TEACHERS

(1) *Introduction*

This brief report has been prepared for the IUPAC Committee on the Teaching of Chemistry by Prof. J. A. CAMPBELL, who is a member of the Committee. It is based on a more detailed report prepared for the Committee by Prof. PAUL O'CONNOR of the University of Minnesota (USA), which surveys the education and in-service training of chemistry teachers in five countries—Germany, Great Britain, India, Japan and the USA.

The problems identified in the O'Connor report and in the brief report that follows are thought to be sufficiently general, not only in the five countries mentioned above but also throughout the world, that a number of recommendations, *listed at the end of the report*, are submitted for wider distribution through national adhering organizations to educationists in general and particularly to those in Ministries of Education and Institutes of Education.

(2) *The general problem*

Many, if not most countries, are faced with a shortage of competent science teachers. Part of this shortage corresponds to the perpetual lack of highly competent people in every field, part results from the current population "explosion" with its growing percentage of school pupils, part is due to the increasing variety of posts available to educated persons, and part to the increasingly rapid obsolescence of scientific competence in the absence of contact with active scientists. The first effect we will never remove, the second may be minimized in the future if population growth becomes better regulated, the third may stabilize as we approach a new sociological steady state. But for the last there is no cure implicit in a wait and see approach.

This shortage of competent science teachers has now existed long enough in many different regions and has been attacked from sufficiently varied approaches that rather definite suggestions can be made to ameliorate the problem on a much wider scale than so far achieved.

No kind of talent is evenly distributed and it is surprisingly common to find that individuals who are excellent teachers are well endowed with other talents as well. One result is their appointment to non-teaching positions of "greater responsibility" and better pay. Few would deny the good teacher access to these positions, but it seems folly for an educational system to put a premium on leaving teaching.

Much of the best teaching is highly individualistic. There are some who claim that great teachers impart a much higher proportion of enthusiasm and insight than they do facts and information. They teach more to encourage students to search for questions than to frame answers, to acquire a visceral involvement in gaining wisdom rather than to make Pavlovian responses. Yet many school systems have such full syllabuses, such demanding detailed examinations, and such a high pass level, that even the best teachers are hard put to exercise their full talents. It is highly likely that if all teachers were given the opportunity for individual emphasis in their courses, the courses would generally improve.

Every country seems to be fortunate in having certain schools recognized as exceptional in their excellence. Yet these schools are held to the same syllabuses and examinations as others . . . syllabuses and examinations that are really designed to set minimum standards. One result is that there is

little opportunity for continual consideration of curriculum reform. Only when a syllabus becomes intolerably out-dated are real changes seriously considered. It may be desirable therefore for every country to select certain schools recognized for outstanding results and release them from any national syllabus and external examination requirements for periods of about three years at a time. These schools would use these periods to experiment with curricular changes and so ensure continual progress in the nation as a whole. During this period these schools would devise their own criterion for assessing their students in the terms normally used.

(3) *The growing school population*

Almost every country is faced with an unusually rapid growth in school attendance due to the combination of high birth rates, and the increased drive for literacy. Both of these demands will level off sometime in the future, but the next twenty years, at least, will provide few breathing spells. The pressure in science education will be at least as great as in other areas, both to produce scientists and to produce scientifically literate societies capable of understanding and controlling the technical factors which so powerfully affect the societies.

Many countries have launched major programmes to explore more effective materials and methods for teaching of science. New textbooks, more interesting and instructive experiments for students, more pertinent classroom material and experiments for the teacher, motion picture films to bring otherwise unavailable systems into the classroom, succinct programme material to help students to learn with minimum supervision, background readings especially for the talented students, are all becoming available. Each helps to present science in a more direct, more exciting, more realistic and more rewarding way, and enables the teacher to teach more efficiently.

Yet none of these techniques changes the ever-rising numerical ratio of enrolling students to available teachers. The number of students in science must be controlled and/or the number of teachers increased.

(4) *The supply of teachers*

For the last 20 years an increasing number of countries have had difficulty in finding teachers. Most countries find that the average formal education of the teachers trained has been dropping. This may not always indicate the teachers are on average worse teachers, but it is hardly cause for joy either. Indeed, some countries which have kept rather careful records on teacher qualifications are convinced that quality has fallen on average. Some are also alarmed at the small percentages of college students with interest in entering teaching.

One might well have predicted both a qualitative and quantitative drop in those wishing to teach as more and more different posts become available to educated people. Any such trend has almost certainly been exacerbated by the generally increased student load, average decrease in student ability, general deterioration of school facilities (especially when compared to the general improvement in other working conditions) and the relative rise in prestige (compared to teaching) of many of the new professions and skilled, or even semi-skilled, occupations. Those countries which seem to have had the least effects in decreasing interest in teaching seem to be those in which the school buildings are best designed, the teachers pay and working conditions compare best with other white collar jobs, the society's interest is highest in education for its children, and the educated person has marked advantages in adult life.

We are not so brazen nor uninformed as to recommend to countries which are just moving in the direction of general education for all that enormous

outlays be made on school facilities, the establishment of multitudinous white collar jobs, or the glorification of teachers. In many of these countries the drive for education and dedication of the teachers is so great that successful schools are held with only minimum protection from the weather. But there do seem to be a large number of nations with large educational systems where little attention has been paid to the relative amenities available to teachers and students compared to other workers. In some cases, indeed, countries with long established educational systems, having a distinguished past, are faced with the biggest drop in teacher supply, both in quantity and quality.

One situation to bear in mind continually is that every student is intimately acquainted with the outward aspects of a teacher's position . . . he has spent many years observing. He can probably make a more intelligent choice with respect to this profession than any other profession in the world. If there is a fall off in quality and quantity of interest in teaching it can hardly be blamed on ignorance of the nature of the profession.

(5) *The obsolescence of teachers*

It is interesting to note that an appreciable number of present teachers went to school and began their teaching when a classical education was by far the most sought after. The subjects and their teaching had been polished by years of dedicated and highly talented teachers. The primary sources were well known, and amply annotated. Obsolescence of knowledge was minimal. In a longer time span, it is probable that an educated person from the fourteenth century could have conversed easily had he returned in the seventeenth, although he would be pleasantly surprised at the spread in intellectual interest. But how many educated persons from the nineteenth century could easily enter a twentieth-century conversation, or even a twentieth-century home?

All forms of education have changed and even the classics are newly annotated. But obsolescence par excellence and rampant actually characterize the sciences. The amount of information, ideas, and conceptual frameworks available to a student entering secondary school doubles while he proceeds to his highest degree, and increases again eight fold during his professional life. It is being predicted that this rate will decrease rapidly in the near future. But it is wise to remember the similar predictions at the end of the nineteenth century. However, levelling off or not, obsolescence is currently a fact of scientific life for teachers.

The problem is not so much that our ideas change from wrong to right ones, as that they shift from very incomplete to more complete, from less general to more general, from less useful to more useful. The secondary school teacher in many countries is especially liable to scientific obsolescence. In most countries he presents the first specialised, subject-oriented materials which are directly related to the current state of the field rather than presenting general tools as is common in elementary education. And subject-oriented materials change rapidly.

Furthermore the secondary school teacher is often professionally alone in his school, isolated from contact with scientists actively engaged in research and in professional discussions of the state of their field. The secondary school teacher is intellectually isolated, and his isolation is made worse by a heavy commitment to teaching which denies him time to stay abreast by reading. And of course, reading, at best, is out-of-date and less satisfying than direct contact in any case.

The gap between the centres of growth of scientific knowledge and the secondary school teachers of the subject is enhanced in most countries by the nature of textbooks for schools and the great gulf between the universities

and the secondary schools. In some cases, the gulf is bridged only by torrid comments from the university professors on the preparation their students received before university entrance. Yet candor would seem to indicate that the real faults tend to lie in the university. After all, the universities trained the secondary school teachers in the first place, approved their syllabuses and examinations in the second place, and refused to spend time on solving the problems in the third place.

An increasing number of countries have effectively broken this university-secondary school barrier in the last ten years. Results are beginning to appear, and they are sometimes dramatic. There are many who would say this recognition of the common interest in educational problems and the establishment of joint efforts in their solution is one of the greatest changes to occur in education in some time. (See Recommendations A and B.)

(6) *In-service training of teachers*

The establishment of contacts between the practising scientist and the secondary school teacher will go far to end the intellectual and professional isolation of the teacher (as well as to acquaint the scientist with some of the problems of effectively communicating his discoveries to others). Probably the most needed and most immediately rewarding area is in-service training for established teachers.

Many countries will claim to have such programmes already, but most of those we have found consist of sessions of one day to one week about once a year and based on a series of lectures on recent discoveries. Stimulating as these are to the teacher, they often have little effect on his classroom. Far more effective in proportion to the time and effort involved are programmes of 4 to 10 weeks consisting of a connected lecture-laboratory-discussion programme on a well-defined area of chemistry.

The most effective courses we have discovered might be labelled "Elementary Chemistry from an advanced point of view". The systems studied are those the teacher will discuss in his own classroom, the experiments done are those his students will do, the questions discussed are those he will discuss in his school. Yet all of these are investigated on a deeper and more thorough level than will be needed with any but the most talented students. The object is to provide the teacher background in depth, not to supply him with set speeches to make to his students.

The 4- to 10-week course allows real involvement and exploration in depth, real laboratory investigation and close contact between the university and secondary school personnel. None of these is possible in the shorter sessions.

A typical daily programme would involve a group of about 50 participants at a lecture, followed by an hour or two of discussion. The rest of the day would find the participants in the laboratory performing experiments, most of which they might wish to try in their own schools. The emphasis would be on presenting chemical ideas in a context which is directly applicable to secondary school problems. Perhaps once or twice a week special lecturers discussing their own special interest and research, would be present. But the emphasis would be on a small number of lecturers presenting a coherent, integrated, extensive study of a particular area of chemistry applicable to the secondary school.

In some cases much of the merit of the longer sessions may be achieved by weekly meetings of not less than half a day each week, as long as the meetings last at least through one term and are all related to a single area and include laboratory work. Such a programme may be especially effective for schools in the immediate vicinity of a university and ensure almost continual

contact in a manner to remove very effectively the isolation felt by many secondary school teachers.

In addition to concentrating on a particular area of chemistry, in-service programmes should emphasize the availability of journals, curriculum materials, examinations, motion pictures, other visual aids, and encourage teachers to try various uses of these in their classrooms. (See Recommendation C.)

Realistic planning for in-service training might take cognizance of the experience in countries which have used them for some years. For example, in the USA half of the 25000 chemistry teachers have not tried to go to an in-service institute in the last ten years, about 15% have tried to go but have not been accepted, and the other 35% have averaged about two institutes each. A fair generalization, based on other countries as well, might be that about one-fourth of teachers are so poorly prepared and so unmotivated that they will neither try to attend or profit much if forced to attend. About half will go with minimum enthusiasm, but perhaps half of these will profit appreciably. The other 25% will profit greatly and will appreciably affect a majority of other teachers who would not themselves derive much from the programmes. The net effect will probably be major improvement in about one-third of all science teachers, some improvement in another third, and little improvement in the final third.

- (7) *Examinations in chemistry (see also the IUPAC report on "The Effect of Examinations in Determining the Chemistry Curriculum up to the Level of University Entrance") CR XXIV, p. 95 ff.*

If teachers attend in-service programmes and become excited by them, the teacher is often frustrated when he returns to his school to the same syllabus, the same text, and the same examinations (often external) as ever. The syllabuses, texts, and examinations must also undergo continual revision.

It is probable that the easiest way to ensure continuous progress and change is to change the examination questions, whether internal or external. Unfortunate though it may be to many, it still seems true that the great majority of teachers and students are exam-oriented. If this is true, syllabus revision should concentrate on examination revision rather than on textbooks or syllabuses. (See Recommendation D.)

Chemistry teachers do have some problems peculiar to their countries, but the science is, in general, the same internationally. An outsider, not involved in local syllabus problems might provide valuable insights into the chemical validity of examinations question at very small cost. It is highly desirable that the commentator be supplied with suggested answers as well. After all the level of answer expected may well be more significant than the phraseology of the question. (See Recommendation E.)

- (8) *The pre-service education of teachers*

Concentrating on the continuing education of teachers is, perhaps, the most rapid way to enhance the current effectiveness of teachers, and there is little likelihood that science will ever reach the situation where continuing education will cease to be important. But one of the current reasons for continuing education is the deficient initial education of many teachers. Part of this is due to the shortages of teachers over recent years, but part is due to the courses teachers followed at universities. Most of these courses should be seriously examined in terms of their adequacy.

In most of the countries with long-established education in science at secondary school level an average of about two-thirds of the teachers seem to have paper qualifications in terms of courses taken and grades achieved,

that should guarantee adequate scientific background. But, actually, perhaps half of these teachers feel very insecure in their professional knowledge. The reasons for their insecurity vary from background to background.

Perhaps one problem is that many universities, even quite prestigious ones, have their introductory courses taught by the least competent chemists in the department, or by competent chemists who are uninterested in introductory chemistry. In fact, the introductory courses are probably the most important courses in any department. They deserve the best, most interested and most interesting teachers.

Advanced courses are usually designed to emphasise research and applied chemistry. The student is encouraged to learn the material as efficiently as possible, using maximum mathematical symbolism. The ideas he is learning are most important to an understanding of chemistry at the secondary school level as well, but few people can rephrase the ideas so that they will be useful at lower levels. Entropy learned in terms of heat engines will hardly be useful in interpreting driving forces for reaction in discussions in secondary schools. Yet surely entropy discussions would allow us to give the student much deeper insights than have been typical in the past. Similar examples abound.

Many countries have teacher training institutions in which a high percentage of their secondary school science teachers are educated. It would seem advisable if they could offer a course, at least one term in length, very similar to that outlined in our discussion of in-service programmes, that is to say a course in "Elementary Chemistry from an advanced point of view". This should be in the last year, and should build on all previous courses. It should go through a good secondary school text and laboratory programme with the teacher actually doing and improving the student experiments. Class discussions would involve ideas to be presented in school in terms of what he has learned at the university. The emphasis again would be on providing the teacher with real insight into elementary problems in the school context. Rather than write more texts for such courses (and none seems to exist), reliance on articles in national publications on chemical education such as the *Journal of Chemical Education*, *Education in Chemistry*, "New Trends in Chemistry" (biennially from UNESCO), "Chemistry Today—a Guide for Teachers" (OECD), *Royal Institute of Chemistry Monographs and Lecture Series*, etc., should provide an excellent set of references. (See Recommendation F.)

(9) *Recommendations*

The following recommendations are submitted:

- A. That top-flight scientists in every college and university acquaint themselves with the situations in science teaching in the secondary schools of their locality. (See Section 5.)
- B. That, having gained such insight, these scientists offer their services and an appreciable fraction of their time to their university, government, and secondary schools to assist in (a) continuing education of secondary school teachers, (b) preparation, testing, and improvement of texts, experiments, examinations, teacher oriented articles, films, equipment, and facilities in secondary schools, (c) the continual modification of emphasis and content in beginning science courses to provide an adequate introduction for non-science students and a sufficient background for those who will continue in science, (d) active encouragement of their own students to teach (even at the expense of less research) while at the university and to consider teaching as a profession. (See Section 5.)

- C. That an intensive programme of in-service institutes be held consisting of explorations of a specific area of chemistry by means of lectures, discussion, and laboratory work in a context directly applicable to teaching in a secondary school. It is considered that these institutes will be most effective if they are staffed by a relatively small permanent staff of good chemists with a sound knowledge of education and if they are associated with a university department of chemistry from whose staff they would draw for lectures. Such institutes should last at least four weeks, and each teacher should be expected to spend about three months in attendance in every five- to seven-year period. Subventions covering the total cost of attending the institute are highly desirable and, in any case, the teacher's travel expenses should be paid and no costs other than board and room be borne by the teachers. Satisfactory completion of an institute should lead to increased emoluments or chances of promotion. (See Section 6.)
- D. That a group of top-flight chemists and secondary school teachers be convened in each country to discuss their examination schemes and some to propose examinations which adequately examine, in terms applicable to secondary school chemistry, student knowledge of the ideas, facts, and conceptual frameworks which chemists actually use. We suggest these questions emphasize gaps of chemical information and concepts as shown by ability to apply them to new situations rather than to simply recall them in the context of some past classroom or textual or laboratory discussion. (See Section 7.)
- E. That, especially in the case of national and widely administered external examinations, the administrators of such exams solicit comments of outstanding professional chemists and secondary school teachers from outside their own country. (See Section 7.)
- F. That institutions educating secondary school science teachers ensure that their introductory courses are given by the best teachers in the institution and that an appropriate course in the final year covers a whole programme in secondary school chemistry from an advanced point of view. (See Section 8.)

INFORMATION AND REPORTS ON IUPAC MEETINGS

Inter-Divisional Committee on Nomenclature (ICN)

*Minutes of the 2nd Meeting held on Thursday, 31 August 1967,
at 14.00 h, at the International Hotel, Prague*

Present: Prof. K. A. JENSEN (Convenor); Prof. R. BELCHER (Recorder); Prof. P. E. VERKADE; Prof. M. L. MCGLASHAN; Dr G. WADDINGTON; Dr G. M. KLINE.

(1) The report from the Division of Organic Chemistry had been circulated to the relevant Commissions and Committees. Dr WADDINGTON asked if four more copies could be made available to him.

(2) The draft manual on Physical Chemical Symbols and Terminology was now due to appear in the Bulletin.

(3) There was some discussion concerning the stage at which the Inter-Divisional Committee should receive tentative reports and it was agreed that it should see these before they were prepared for publication in the Bulletin. The Chairmen and Secretary of the relevant Commissions should receive a copy each.

Dr WADDINGTON in a letter to Prof. BELCHER (12 November 1965) had commented on the various stages through which reports pass and had made suggestions. Prof. BELCHER has passed these on to the late Dr DEGENS but had had no reply before the latter's untimely death.

(4) It was agreed that there were many problems in the nomenclature of polymer chemistry and it was essential that close contact should be maintained between the organic and polymer sections.

(5) Prof. JENSEN considered that representatives of the Inorganic, Organic and Polymer Nomenclature Commissions should meet at the next Conference. It was agreed to try to arrange this meeting.

It was also pointed out that there was still some usage of old names in the literature of industrial chemistry and the attention of the Applied Chemistry Division should be drawn to this fact. Prof. VERKADE was not sanguine that this would have any effect.

(6) The Report on "Terminology and Symbols in Colloid and Surface Chemistry" submitted by the Commission on Colloid and Surface Chemistry had been received by the Recorder. There had not been time to circulate this before the Prague meeting but it had been notified to his Commission during its first session. Prof. SAMUELSON of the Nomenclature Commission, Analytical Division, had asked for the copy as he felt it would be of use to him in his present project on Terminology in Chromatography.

(7) Prof. BELCHER reported that he had followed up the request of the Committee in arranging for a compilation to be made of trivial names used for reagents in analytical chemistry. This project had been started by Mr FENNELL and so far 300 reference cards had been compiled. However, Mr FENNELL had now been elected as Divisional Secretary and so could not continue this task. It had been taken over by Prof. IRVING. Prof. JENSEN remarked that the Inorganic Division might deal with non-analytical trivial names.

It was also remarked that it would be useful if the Physical Chemistry Section could supply a list of abbreviated terms used to Prof. JENSEN for definition.

Prof. BELCHER remarked that various letters had been received and circulated to the Committee. These are listed below for reference:

From C.J. KEATTCH, 10 June 1966, *Re*: Thermal Analysis Nomenclature. Acknowledgement by Prof. BELCHER. Letter from Dr WADDINGTON to KEATTCH, 13 October 1966.

From Dr K.L. LOENING, 5 August 1966. *Re*: "Naming and Indexing of Chemical Compounds from Chemical Abstracts". This project in progress.

From C.J. KEATTCH, 11 January 1967. *Re*: a sub-committee of ICTA which is to deal with selection of materials for analytical standards in DTA and TC. A meeting was due October 1967. No specific date was mentioned and no further information was available.

Prof. BELCHER also asked that several reports from his Commission had reached the Bulletin stage too late for circulation to the ICN. Some new reports were shortly due and so would be made available.

A massive report on "Quantities and Units in Clinical Chemistry" had been received from Dr R. DYBKER of Copenhagen (3.4.67) asking for comment by Prof. BELCHER. Time was very limited because comment was required in time for publication before the Prague meeting. Prof. BELCHER felt he was unqualified to comment on the document and passed it over to one of the leading clinical chemists in Birmingham. The latter, however, stated later that as British Clinical Chemistry opinion had been expressed already it would be out of place to comment. Nevertheless some ambiguities were pointed out and notified to Dr DYBKER.

(8) Dr WADDINGTON asked if it was felt that there was sufficient knowledge of IUPAC documents. Although the Committee considered that IUPAC documents were often overlooked, there was no suggestion how to remedy this matter.

(9) Dr KLINE asked if a report published in the *Journal of Pure and Applied Chemistry* could be copied. Prof. JENSEN said the whole purpose of IUPAC work was that it should be ready available to all; in principle it was wrong that we should have to ask permission to reproduce IUPAC documents.

At this stage Prof. BELCHER had to leave to attend a meeting of the Executive Committee of the Analytical Division and Prof. JENSEN continued with the recording.

The Committee was somewhat concerned about the circulation and availability of the nomenclature rules. While opinions were divided concerning the desirability of having the nomenclature rules copy-righted, it was agreed that translation, quotation and photocopying of the rules should be facilitated in every way. Prof. JENSEN was requested to discuss this problem with the Chairman of the Editorial Board, Prof. H.W. THOMPSON.

The meeting ended at ca. 16.00 h.

II.1 COMMISSION ON ATOMIC WEIGHTS

Information Notice No. 3/67

(1) This notice is sent to all former and new titular and associate members of the Commission.

(2) Although the Commission did not meet during the Prague 1967 IUPAC Conference, its business was transacted thanks to the assistance of the IUPAC Secretary General, and to the exertion of members, in particular Dr CAMERON who drafted the report, and of Prof. THODE who, being present in Prague, steered our affairs through the IUPAC Division of Inorganic Chemistry.

Most of the following notes are quotations or summaries from a letter from Prof. THODE to the Commission's secretary, dated 5 September 1967.

(3) "It was pleasure" (writes Prof. THODE) "to present the report of the International Commission on Atomic Weights to the Inorganic Division of IUPAC meeting in Prague. The report included the report prepared by CAMERON and the tables of radioactive isotopes prepared by K. WAY."

"The report was well received and the Commission was congratulated on its ability to conduct business by mail. I indicated that the final report for publication would be ready between 15 and 30 September."

"Dr DE BOER and President KLEMM singled out Dr WICHERS for honorable mention as chairman of the Commission. Dr DE BOER in his council report emphasized the *permanent* nature* of the Commission on Atomic Weights and expressed his appreciation and thanks to the members of the Commission and particularly to Dr WICHERS, its chairman, for the excellent work they are doing."

"I indicated to the Division that there would be a new table of atomic masses prepared next year and that the new values could lead to recommended changes in atomic weights. I also mentioned the report I am preparing on the variations in atomic weights due to variations in the isotopic composition of the elements in nature. Finally, I pointed out that new determination of absolute abundances which appear each year will also lead to changes in atomic weights from time to time. The feeling was that there would be work for the Commission for a few years and that it would be profitable for us to hold a meeting at the IUPAC conference in Rome in 1969. The Council approved the Division report and the Bureau budgeted for a Commission meeting in 1969."

(4) After incorporating the latest additions and corrections, the 1967 Report and the 1967 Tables are being sent to the IUPAC General Secretary as appended to this Notice.

(5) The Division of Inorganic Chemistry, by election, established the following membership for our Commission:

Titular members

1967-1971	Dr E. WICHERS	Dr J. SPAEPEN
	Prof. S. FUJIWARA	Prof. H. G. THODE
	Prof. N. H. GREENWOOD	Prof. A. H. WAPSTRA
	Dr H. S. PEISER	1967-1969 Dr J. GUÉRON

Associate members

Dr A. A. CAMERON	Prof. E. ROTH
Prof. G. N. FLEROV	Dr H. J. ŠVEC

A list of addresses was annexed to this Notice. Members were kindly requested to send me promptly any amendments necessary to the circulation of a final list.

(6) Dr WICHERS, as Chairman of our Commission, was elected, with high praise, as a member of the IUPAC Division of Inorganic Chemistry.

J. GUÉRON, Secretary

* "I had an informal discussion with Prof. KONDRATIEV, the new IUPAC President, and he wondered why it was necessary to have both an international Commission on Atomic Masses IUPAP, and one on atomic weights IUPAC. I pointed out that there was good liaison between the two Commissions but perhaps some thought could be given to the matter."

SYMPOSIUM INTERNATIONAL DE CHIMIE MACROMOLÉCULAIRE

Bruxelles-Louvain, 12-16 juin 1967

Dans le cadre des activités de la Commission de Macromolécules IUPAC, un Symposium international de Chimie macromoléculaire a été organisé sous les auspices de IUPAC à Bruxelles et Louvain du 12 au 16 juin 1967 sous la présidence du Prof. G. SMETS de l'Université de Louvain. Le thème général du Congrès était: «*Organic chemistry and internal structure of synthetic high polymers*».

Cinq conférences plénières ont été données, à savoir:

- C. E. H. BAWN (GB): New methods of polymerization
- A. KATCHALSKY (Isr.): Transport and exchange phenomena in synthetic polymers
- H. MARK (USA): Synthetic polymers and their relation to biochemistry
- I. SAKURADA (Japan): Some fundamental aspects of polymer reactions
- V. A. KARGIN (URSS): Supramolecular structures in polymers in relation with their synthesis and chemical structure

tandis que 10 conférences principales et d'introduction aux discussions ont été présentées par:

- A. A. BERLIN (URSS): Advances and trends in the chemistry of polymers with a conjugated system
- F. A. BOVEY (USA): Nuclear magnetic resonance and optical studies of polypeptide chain conformation
- H. P. GREGOR (USA): Selective membranes
- N. GRASSIE (GB): Polymer degradation and ESR
- S. KRIMM (USA): Infrared spectroscopy and polymer structure
- C. S. MARVEL (USA): Thermostable polymers
- S. OKAMURA (Japan): Cationic polymerizations of $\alpha\beta$ -disubstituted olefins
- P. PINO (Italie): Optical activity and rotatory dispersion in synthetic polymers
- P. REMPP (France): Synthèses et structures nouvelles de polymères
- R. C. SCHULZ (DBR): On new chemical reactions of polymers

Le nombre de communications a été limité intentionnellement afin de réserver le plus de temps possible aux discussions et de garder les groupes de travail aussi homogènes que possible. Les communications étaient groupées en 10 sections différentes; leur nombre s'élevait à 92.

La séance d'inauguration avait été rehaussée par la présence de M. F. GROOTJANS, ministre de l'Education nationale qui a présenté un discours de bienvenue à l'Assemblée (900 participants).

La présidence d'honneur du Congrès était assurée par M. J. SOLVAY, tandis que les présidents d'honneur du Comité scientifique étaient le Prof. G. NATTA, prix Nobel, et O. WICHTERLÉ, président de l'actuelle Division Macromoléculaire IUPAC.

L'ensemble des communications présentées au Congrès sera publié dans un tome spécial du *Journal of Polymer Science* (Série C), alors que les conférences plénières et principales paraîtront dans un tome spécial de *Pure and Applied Chemistry*.

G. SMETS

IIIRD INTERNATIONAL SYMPOSIUM ON ORGANOMETALLIC CHEMISTRY

München (Germany) 28 August–1 September 1967

The IIIrd International Symposium on Organometallic Chemistry was held at the Technische Hochschule München (Germany) from 28 August–1 September 1967. The meeting was organized by the Gesellschaft Deutscher Chemiker under the sponsorship of IUPAC, Prof. E.O.FISCHER acted as chairman of the Organizing Committee.

The scientific programme included 5 plenary lectures—the texts of which will be published in *Pure and Applied Chemistry* and which were given by Prof. M.F.HAWTHORNE, Prof. A.NESMEYANOV, Prof. P.L.PAUSON, Prof. R.PETTIT and Prof. G.WILKE—, and about 180 discussion papers in three parallel sessions. More than 500 participants from 22 countries actively attended to the lectures as well as the discussions.

The main topics of the symposium were reports on novel synthetic routes to the formation of metal-carbon bonds, reactions of organometallic complexes and various physico-chemical investigations on these compounds. The theoretical treatments of substances of general interest to the auditorium were dealt with to some extent also.

E. O. FISCHER

XTH INTERNATIONAL CONFERENCE ON COORDINATION CHEMISTRY

Tokyo and Nikko, 12–16 September 1967

The Xth International Conference on Coordination Chemistry (X.ICCC) took place in Tokyo and Nikko (Japan) from 12–16 September 1967. It was organized by the Chemical Society of Japan under the sponsorship of the Science Council of Japan and the International Union of Pure and Applied Chemistry. The Organizing Committee was composed of 32 members under the chairmanship of Prof. YUJI SHIBATA, President of the Japan Academy.

The program covered a wide field of coordination chemistry, including the chemistry of organometallic compounds.

The Opening Ceremony was held in the morning of 12 September, Tuesday, in the Tokyo Metropolitan Festival Hall, Ueno Park, Tokyo. The Chairman of the Organizing Committee, Prof. SHIBATA, gave an opening address, followed by the welcoming address of Prof. H.SUGINOME, President of the Chemical Society of Japan. After these two addresses given in English, Prof. S.TOMONAGA, President of the Science Council of Japan, delivered his greetings in Japanese. As the last speaker of the Opening Ceremony, Prof. J.C.BAILAR, Jr., Treasurer of the IUPAC, talked on the activity of the International Union of Pure and Applied Chemistry.

After the Opening Ceremony following three plenary lectures were delivered in the same Festival Hall.

- Prof. H.S.NYHOLM (UK): Magnetism, bonding and structure of coordination compounds
- Prof. G.WILKE (Germany): Transition metal complexes in organic chemistry
- Prof. FRED BASOLO (USA): Mechanism of substitution reactions of metal complexes

When these three plenary lectures were finished at about 15.00, all the participants moved by a special train to Nikko, a summer resort which is situated about 100 km to the north of Tokyo. It took about two hours, and after arrival in Nikko a "mixer" was held in the same evening in the Nikko Kanaya Hotel. Most of the overseas participants stayed in this hotel where the Conference was held.

From the morning of 13 September, Wednesday, till the afternoon of 16 September Saturday, three parallel sessions were held simultaneously in three rooms of the Nikko Kanaya Hotel, and 117 papers were presented. For each paper 25 minutes were allotted including time for discussion. These sessions were all well attended and the discussions were quite lively.

The topics and speakers of the five plenary lectures delivered in Nikko were:

- Prof. L. G. SILLÉN (Sweden): Some recent results on hydrolytic equilibria
- Prof. YOSHIHIKO SAITO (Japan): Structures and absolute configurations of cobalt (III) complexes
- Prof. O. A. REUTOV (USSR): On the importance of coordination in electrophilic substitution reactions of organometallic compounds
- Prof. L. SACCONI (Italy): Five-coordination in 3d metal complexes
- Prof. A. E. MARTELL: Catalytic effects of metal chelate compounds

All the plenary lectures are to be printed in the IUPAC journal, *Pure and Applied Chemistry*, and published as a specially bound reprint from Butterworths, London, in 1968. Abstracts of papers presented in the X.ICCC were printed by the photographic reproduction method and thus prepared "Proceedings of the Xth International Conference on Coordination Chemistry" were distributed to the participants.

Besides the academic program a welcoming party for the overseas participants was held by Prof. H. SUGINOME, President of the Chemical Society of Japan, in the evening of 11 September in Tokyo. In Nikko an excursion to the Lake Chuzenji and a closing banquet were held in the afternoon of 14 September, Thursday, and in the evening of 16 September, Saturday, respectively.

There was also a program for the ladies accompanying active members. This included a trip from Nikko to Mashiko which is a pottery making town. Meetings for the demonstration of tea ceremony and flower arrangements were also held in Nikko. It was unfortunate that during the whole Conference period the weather was rainy except for the afternoon of the excursion.

The Conference was adjourned in Nikko in the morning of 17 September, Sunday, but on 18 September, Monday, a post-conference activity, Scientific Visits, were held in Tokyo which included the visits to the chemistry laboratories of the University of Tokyo, office of the Chemical Society of Japan, the Canon Camera Factory and a boat trip from the Kawasaki pier to Yokohama along the Industrial Coast of the Tokyo Bay.

The Conference was well attended by 123 overseas members from following 22 countries, accompanied by 47 family members, and 276 Japanese members: Australia, Brasil, Canada, Denmark, France, Germany, Hong Kong, India, Israel, Italy, Korea, The Netherlands, New Zealand, Poland, Rumania, Sweden, Switzerland, Republic of China, Thailand, United Kingdom, USA and USSR.

The next ICCC will be held in September 1968 in Israel. Information about it will be available from Prof. M. CAIS, Technicon—Technical Institute of Israel, Haifa, Israel. Those who wish to obtain "Proceedings of X.ICCC" are requested to write to the X.ICCC, Chemical Society of Japan, 1-5 Kanda-Surugadai, Tokyo. The price is \$5.00 plus postage.

K. YAMASAKI, General Secretary of the X.ICCC

DETAILED INFORMATION REGARDING FORTHCOMING MEETINGS

International Atomic Energy Agency

IIIRD CONFERENCE ON PLASMA PHYSICS AND CONTROLLED NUCLEAR FUSION RESEARCH

Novosibirsk (USSR), 1-7 August 1968

Since the Second United Nations Conference on the Peaceful Uses of Atomic Energy (Geneva, 1958), the achievement of the controlled release of fusion energy has become the goal of active research programs in many countries. The challenging problems of production and confinement of hot dense plasmas have given rise to steadily expanding theoretical and experimental efforts. This growth in research activity is accompanied by an increasing need for the international exchange of scientific results and information.

In acknowledgement of this need, the International Atomic Energy Agency is now organizing its IIIrd Conference on Plasma Physics and Controlled Nuclear Fusion Research. The first and second conferences of the IAEA series were held at Salzburg in 1961 and at Culham in 1965. The Agency also contributes to the progress of fusion research by publishing the journal "Nuclear Fusion".

List of topics to be covered by the Conference

The following topics will be covered:

- (a) General theory of plasma confined by magnetic and electromagnetic fields
- (b) Experimental and theoretical problems concerned with:
 - (i) Plasma confinement
 - (ii) Plasma compression, heating and acceleration
 - (iii) Plasma instabilities
 - (iv) Plasma waves and oscillations
 - (v) Turbulence and non-linear phenomena
 - (vi) Diffusion
 - (vii) Shock waves in plasma
 - (viii) Plasma and particle injection
 - (ix) Interaction of particles and radiation with plasma

**International Atomic Energy Agency and
Joint Commission on Applied Radioactivity, etc.**

INTERNATIONAL SYMPOSIUM ON METEORITE RESEARCH

Vienna (Austria), 7-13 August 1968

A great deal of interest has always been attached to meteorites. In ancient times their fall was often considered to be a sign from heaven. It has been estimated that hundreds of tons of solid substance from space reach the earth every day, most of which is vaporized in the atmosphere. Only a few hundred pieces are large enough to reach the solid surface of the earth and of these only a few are recovered.

Meteorites are of extraordinary scientific value and research on them cuts across many scientific disciplines: astrophysicists, cosmologists, nuclear physicists, metallurgists and chemists consider them legitimate objects for their investigations. With their aid we can obtain useful information relevant to the history of the universe and to the original elemental and isotopic composition of matter. We may even hope to receive some indication concerning the possibility of extra-terrestrial life. Meteorites are also useful as natural space probes for determining cosmic radiation density along their path through the solar system: both spatial and temporal variation in cosmic radiation may be investigated with their help. It goes without saying that the measurement of cosmic-ray induced radioactivity in meteorites provides this information at a fraction of the cost required for sending artificial probes into space.

The symposium will be concerned with all these aspects of meteorites—with their origin, history, orbital characteristics, composition, structure and radioactivity. It will be truly interdisciplinary in that it will bring together scientists of quite different training and outlook who have a common interest in meteorites.

THIRD INTERNATIONAL FERMENTATION SYMPOSIUM

New Brunswick, NJ (USA), 2-6 September 1968

Institute of Microbiology, Rutgers—The State University,
New Brunswick, New Jersey, USA,
sponsored by Division of Microbial Chemistry and Technology,
American Chemical Society; Fermentation Industries Section;
International Union of Pure and Applied Chemistry

Invitation

Attendance is open to all scientists interested in fermentation technology and related fields.

Scientific program

The theme of the program is: Fermentation Advances in the Light of Recent Theoretical Progress in Microbiology, Biochemistry and Engineering.

The program will have two plenary sessions, each of which will have two invited speakers. The sessions will be devoted to (1) the evaluation of our fundamental understanding of microbial biosynthesis and (2) the practical application of present fermentation techniques as related to world food and health problems.

7 focal topic sessions are being planned. Papers at these sessions will be by invitation of co-chairmen for each focal topic session.

Approximately 40 general papers will be accepted by the program co-chairmen, Dr A.E. HUMPHREY and Dr W.E. BROWN. Some papers will be accepted with a view to encouraging a broad geographical distribution of participants and encouraging the participation of young investigators capable of contributing new ideas in the various sessions.

Accommodations

Arrangements have been made to house registrants in the University dormitories and to have their meals in the University Commons dining hall. Limited space will be available on campus for women and couples. An all-

inclusive registration fee of approximately \$150 (USA) will cover cost of registration, a copy of the proceedings, housing, meals and social activities.

Those who prefer off campus housing may make their own arrangements at local motels and hotels, the names and locations of which will be issued in a future announcement.

Publication

Papers presented at the plenary and focal topic sessions of the Third International Fermentation Symposium will be published in *Pure and Applied Chemistry* shortly after the meetings. To expedite publication, all authors are required to provide 2 copies of their manuscript no later than the time of presentation. Copies of the publication will be distributed in 1969 to all registrants of the Symposium. Copies also will be available for purchase.

Additional Information

Persons desiring additional information on any phase of the Symposium should write to:

Dr ARTHUR E. HUMPHREY,
The School of Chemical Engineering,
University of Pennsylvania,
Philadelphia, Penna. 19104 (USA)
or
Dr WILLIAM E. BROWN,
Squibb Institute for Medical Research,
New Brunswick, New Jersey 08903 (USA)

INTERNATIONAL SYMPOSIUM ON MACROMOLECULAR CHEMISTRY

Toronto, 3-6 September 1968

Second circular

Provisional program

All scientific sessions will be held in the Royal York Hotel. The theme of the Symposium is the Structure and Properties of Macromolecular Systems, including synthetic natural and biological polymers. The program will be arranged in the form of special symposia dealing with selected topics.

The morning sessions will be devoted to invited lectures and the afternoon sessions to contributed research papers. It will be necessary to run concurrent sessions.

The topics that will be discussed are:

- A. Structure and properties of polymers
 1. The thermodynamics of solutions
 2. Conformations of molecules in solution
 3. Polyelectrolytes and their solutions
 4. Elucidation of molecular structure—tacticity and order
 5. Electrical properties—conduction and relaxation processes
 6. Plastic deformation and structure in crystalline polymers
 7. Adsorption of polymers

8. Rheology of polymer composites, blends and suspensions
 9. Reinforced polymers—interfacial phenomena and failure mechanisms
 10. Elastomers—network topology and viscoelasticity
 11. Cellulose, hemicelluloses and lignins—structure and properties
 12. Organic and inorganic glasses—state and transitions
- B. Structure and function of biopolymers
1. Structure and properties of nucleic acids, enzymes and immunoglobulins
 2. Conformations of polynucleotides and polypeptides
 3. Conformational changes on interaction of biopolymers with ligand molecules

Invited Lectures

There will be 4 plenary lectures which will key-note the program on each of the four days of the Symposium. In addition, there will be 32 sessional lectures of a review nature covering various aspects of the major themes.

The following speakers have accepted invitations to present lectures:

H. BENOIT: Centre de Recherches sur les Macromolécules, Strasbourg (France)
 S. BYWATER: National Research Council, Ottawa (Canada)
 J.-P. CHANGEUX: Institut Pasteur, Paris (France)
 M. EIGEN: Max-Planck-Institut, Göttingen (W. Germany)
 G. FELSENFELD: National Institute of Health, Md. (USA)
 P. J. FLORY: Stanford University, Cal. (USA)
 M. GOLDSTEIN: Yeshiva University, New York City (USA)
 K. IMAHORI: University of Tokyo (JAPAN)
 V. A. KARGIN: State University of Moscow, USSR
 H. MARK: Brooklyn Polytechnic Institute, NY (USA)
 R. St. J. MANLEY: Pulp and Paper Research Institute, Montreal (Canada)
 R. H. MARCHESSAULT: Syracuse University, NY (USA)
 S. G. MASON: Pulp and Paper Research Institute, Montreal (Canada)
 D. McINTYRE: University of Akron, Ohio (USA)
 H. MORAWETZ: Brooklyn Polytechnic Institute (USA)
 D. C. PHILLIPS: Oxford University (UK)
 V. T. STANNETT: Camille Dreyfus Laboratory, NC (USA)
 L. STRYER: Stanford University, Cal. (USA)
 G. ZERBI: Milan University (Italy)

Publication

Preprints of the papers to be presented at the Symposium will be distributed to all registrants at the time of the meeting.

Arrangements have been made for the contributed papers to be published in a special issue of the *Journal of Polymer Science*. Authors will be informed of the format required for manuscripts by the Program Committee. It is not inten to publishedd the discussion of papers.

Cable: Macromol, Toronto

Organizing Committee,
 Box 932,
 Terminal A,
 Toronto (Canada)

INTERNATIONAL SYMPOSIUM ON MACROMOLECULAR CHEMISTRY

Toronto (Canada), 3-6 September 1968

The Deutsches Reisebüro GmbH, Sonderdienst für Studien- und Kongressreisen, D-6000 Frankfurt/Main 1, Postschliessfach 3621, Eschersheimer Landstr. 25-27, (Germany), has organized group travel for participants from Germany at a very favourable rate. In other countries, similar projects might be in operation. Scientists interested in this Symposium are kindly invited to take advantage of such group flights.

IUPAC-SYMPOSIUM "VALENCE ISOMERISATION"

Karlsruhe, 9-12 September 1968

A IUPAC-Symposium on "Valence-Isomerisation" will take place from 9 to 12 September 1968, in Karlsruhe (Germany) and will be prepared by the Gesellschaft Deutscher Chemiker. Prof. CRIGEE, who is chairman of the Scientific Committee, invited the following plenary lecturers who will be ready to present their paper:

F. A. L. ANET, University of California
W. VON E. DOERING, Yale University
H. M. FREY, University of Southampton
J. F. M. OTH, European Research Association, Brussels
H. SCHMID, Universität Zürich
R. SRINIVASAN, IBM Watson Research Center
E. VOGEL, Universität Köln
R. B. WOODWARD, Harvard University

On behalf of the chairman, Prof. CRIGEE, we should like to invite you to submit discussion papers *until 15 March 1968*. An abstract of one type-written page in the maximum should be added in five copies. Symposium languages are English, German and French.

MICROSYMPOSIUM ON STRUCTURE OF ORGANIC SOLIDS IN MACROMOLECULAR CHEMISTRY

Prague, 16-19 September 1968

The Institute of Macromolecular Chemistry (Czechoslovak Academy of Sciences) and The Czechoslovak Chemical Society are organizing a Micro-symposium on *Structure of Organic Solids in Macromolecular Chemistry* to be held in Prague, 16-19 September 1968. This conference will be devoted to the structure of macromolecular substances, of low molecular oligomers and of all more complicated organic compounds whose structure is interesting for macromolecular science. The scope is limited by the choice of diffraction methods as the source of information on the structure of organic solids but papers on crystallochemical subjects are not excluded.

The program will include following topics:

Structure of fibres.—Structure of amorphous solids.—Structure of related low molecular-weight compounds.—Instrumentation.—Methods and computations.

The following speakers have agreed to give invited lectures:

W. HOPPE (Germany)	New trends in the structure determination of complex organic compounds
B. K. VAINSHTEIN (USSR)	Structure of fibres
W. O. RULAND (Belgium)	Structure of amorphous solids
C. A. TAYLOR (UK)	Optical methods as an aid for structure determination
J. S. ROLLET (UK)	Computing methods in structure determination

Authors are requested to use preferably English, whenever possible.

Discussions: Facilities will be provided for discussions of a wide range of general and special problems of the distribution analysis and fractionation.

Accommodation will be provided in a student dormitory or at a hotel near the Institute (according to the wish of the participant). Meals will be served at the Institute on Monday, 16 September.

MICROSYMPOSIUM ON DISTRIBUTION ANALYSIS AND FRACTIONATION OF POLYMERS

Prague, 23–26 September 1968

The Institute of Macromolecular Chemistry and the Institute of Physical Chemistry (Czechoslovak Academy of Sciences) in cooperation with the Institute of Physical Chemistry (Charles University) are organizing a Microsymposium on *Distribution Analysis and Fractionation of Polymers*, to be held in Prague, 23–26 September 1968. The Microsymposium will be devoted to the basic problems of the theory and practice of the distribution analysis and fractionation of homopolymers and copolymers.

Topics: Distribution analysis based on phase equilibria in polydisperse polymer-solvent systems (including turbidimetric titration).

Fraction based on phase equilibria (including e.g. effects of crystallinity and stereoregularity; column methods; problems of micro- and macroscale fractionation).—Gel permeation chromatography.—Distribution analysis based on different physical properties of solutions (sedimentation, diffusion, light scattering, etc.).

The 'program will include main lectures, scientific communications and discussions. The main lectures on following topics are intended: Critical review of the fractionation methods.—Phase equilibria in multicomponent systems.—Fractionation of copolymers.—Gel permeation chromatography.—Distribution analysis based on physical properties of solutions.

The following speakers have been invited to give the main lectures:

H. BENOÎT (France)	R. KONINGSVELD (Holland)
A. D. LITMANOVICH (USSR)	J. C. MOORE (USA)
N. J. SCHNEIDER (USA)	and others

Discussions: Facilities will be provided for discussions of a wide range of general and special problems of the distribution analysis and fractionation. Authors are requested to use preferably English, whenever possible.

Accommodation will be provided in a student dormitory or at a hotel near the Institute (according to the wish of the participant). Meals will be served in the Institute cafeteria. An informal dinner will be served at the Institute on Monday, 23 September.

INTERNATIONAL SYMPOSIUM ON NATURAL PRODUCTS; STEROIDS AND TERPENES

21-25 April 1969, México City (México)

Sponsored by Sociedad Química de México, Ciprés 176—México 4, DF, Apdo. Postal 4-875

Number of papers to be presented: 50 to 80

Ten invited lecturers:

Dr K. SCHREIBER
Dr K. TAKEDA
Dr D. H. R. BARTON
Dr C. DJERASSI
Dr G. BÜCHI

Dr R. DEGHENGI
Dr J. ROMO
Dr J. IRIARTE
Dr TOLDI
Dr O. JEGGER

INTERNATIONAL SYMPOSIUM ON ANALYTICAL CHEMISTRY

Birmingham (UK), 21-25 July 1969

The Midlands Section of the Society for Analytical Chemistry is organizing an International Symposium at the University, Birmingham (UK), over the period 21-25 July 1969. The programme will include invited and contributed papers covering a wide field of analytical chemistry, together with social events, a ladies' programme, etc.

Some preliminary notices gave the date of this Symposium as 6-10 April, 1970, but this has now been changed to the above.

General information about the Symposium can be obtained from Mr D. M. PEAKE, Research Department, Imperial Metal Industries Limited, P.O. Box 216, Witton, Birmingham 6 (UK). Information about the scientific programme is obtainable from Dr W. I. STEPHEN, Department of Chemistry, The University, P.O. Box 363, Birmingham 15 (UK).

IUPAC-SPONSORED SYMPOSIUM ON CHEMICAL CONTROL OF THE HUMAN ENVIRONMENT

Johannesburg (South Africa), July 1969

It is planned to hold this in the *third week of July 1969*. Since some of those attending the Symposium may wish to go on to the Conference and Congress in Melbourne in August 1969, on the same round trip ticket, consideration is being given to arrangement of tours to other centres of scientific interest in South Africa after the Symposium.

The subject of the Symposium is to be interpreted broadly as dealing with all chemical topics relating to control of environment. Thus, it is not confined to the use of chemicals for control, but includes all chemical and biochemical problems arising from the use of such chemicals, and also the

isolation, analysis and identification of chemical substances which are injurious and which therefore should be controlled.

Apart from original papers from both South African and other authors, the opportunity will be taken to present a number of review papers on South African work, where this covers conditions which are outside the experience of most workers in other countries.

Owing to the broad nature of the symposium, a large number of papers is expected so that, to remain within the confines of a single week, at least three sessions will be held concurrently, and speakers will be asked to present summaries only. The medium will be English.

For convenience, the Symposium will be divided into five sections, each of which will be introduced by at least one plenary lecture by a leading scientist in the particular field.

In the following, those aspects which will receive particular attention in each section are outlined, and the names of the corresponding plenary lecturers are given.

1 *Control of Air Pollution*

will deal with methods for measuring pollution and with methods for reducing pollution to a minimum.

The plenary lecturer will be Prof. Dr WOLFGANG TESKE, who is head of a group of Farbwerke Hoechst AG, Frankfurt (West Germany), which has carried out much research on control of industrial gaseous emissions.

2 *Control of Water Supplies*

will deal with chemical methods of treatment for water supplies and for reuse of effluents.

The plenary lecturer will be Prof. K. J. IVES, of the Department of Civil and Municipal Engineering, University College, London.

3 *Control of Agricultural Pests*

will deal with insecticides, herbicides and chemical lures such as sex attractants in the broadest possible sense, namely, utilization, control of residues, metabolism, etc.

There are two plenary lecturers, namely, Prof. F. A. GUNTHER, Citrus Experimental Station, University of California, who is an authority on analysis of pesticide residues; and Prof. A. S. CRAFTS, Department of Botany, University of California, whose studies have lain in the field of herbicide metabolism.

4 *Control of Health*

The use of chemotherapeutic drugs for human health has been excluded from the symposium since its implications are too vast to be covered in the limited time available. This section is planned therefore to cover two specific subsections.

- (i) Chemical methods for the control of disease-bearing vectors, particularly those of importance to human health
- (ii) Use of antibiotics in agriculture both to combat disease and to facilitate production

It is expected to have a plenary speaker for each of these topics.

5 *Control of Toxic Substances*

can be regarded as a further subsection of 4, as it is concerned with substances injurious to health, both human and animal. It embraces the many harmful substances which can occur in foodstuffs for human consumption; but, in South Africa, a great deal of work has been done on veterinary

aspects, due to an abundance of poisonous plants and, in more recent years, to toxins of fungal origin.

The plenary speaker is Dr L. A. GOLDBLATT of the Southern Utilization Research and Development Division, of the US Agricultural Research Service, who is an authority on the field of mycotoxins.

7TH CONGRESS OF CLINICAL CHEMISTRY

Geneva, 8-13 September 1969

Number of papers to be presented, and approximate length:

7 Main conferences, about 15 pages each

5 Symposia, abstracted in about 60 pages total

200 Individual papers (abstracts: 280 p. selected papers, 500 pages)

Number of specially invited lecturers (7):

J. B. WILLIS, Australia
L. ORNSTEIN, New York
W. C. PURDY, University
Maryland

S. UDENFRIEND, Bethesda
D. SELIGSON, New Haven
G. SEMENZA, Zurich
L. ERNSTER, Stockholm

SYMPOSIUM INTERNATIONAL D'ANALYSE CONFORMATIONNELLE

Bruxelles, septembre 1969

(susceptible d'intéresser les chercheurs dans les domaines de

- la Chimie organique
- la Chimie organique physique
- la Pharmacie
- la Biochimie)

aura lieu à Bruxelles en septembre 1969 sous la Présidence du Prof. CHIURDOGLU et sous les auspices de la Société chimique de Belgique, de la Fédération des Industries chimiques de Belgique et de l'Université libre de Bruxelles.

VITH SYMPOSIUM ON THE CHEMISTRY OF NATURAL PRODUCTS

Riga, Beginning of July 1970

Number of papers to be presented, and approximate length:

200-300 papers, 2 pages of typescript each.

Number of specially invited lecturers: about 10

Among those to be invited are the following:

Prof. D. H. R. BARTON, UK
Prof. C. DJERASSI, USA
Prof. H. B. KHORANA, USA
Prof. D. E. KOSHLAND, USA
Prof. E. LEDERER, France

Prof. K. NAKANISHI, Japan
Prof. V. Prelog, Switzerland
Prof. F. ŠORN, Czechoslovakia
Prof. L. L. M. VAN DEENEN,
Netherlands

PROVISIONAL IUPAC METHOD FOR AFLATOXIN IN PEANUTS, PEANUT BUTTER, AND PEANUT MEAL

The potential hazard to man from mycotoxins has become more apparent in recent years. This concern stems from the work on the aflatoxins in a number of laboratories throughout the world. The IUPAC recognized the need for adequate methodology with which the interested nations could accumulate data to assess the extent of the problem as it affects their national needs. Consequently the Food Section of IUPAC established the Trace Substances Commission in 1965. The first formal meeting was held in Paris, France, 1 July 1965, and the Commission was charged with two major subject areas; namely, mycotoxins and smoke constituents in food. As a result of several international collaborative studies in the past two years, the Trace Substances Commission has recommended a provisional IUPAC procedure for the determination of aflatoxins B₁, B₂, G₁, and G₂ in peanuts, peanut butter, and peanut meal. The method provides a choice of determinative steps, which allows the analyzing laboratory to choose the step most appropriate for their needs. It is hoped that the publication of this provisional procedure in the "Information Bulletin" will stimulate further work and suggestions for improvements from the international scientific community. The method is based on analytical principles developed in the laboratories of the Tropical Products Institute of England, Lever Bros. of Holland and England, and the United States Food and Drug Administration.

Signed: HENRY FISCHBACH, Ph.D.

Apparatus

- (a) Disc Mill.—Model 4E, Straub Co. (Quaker City Grinding Mills, Philadelphia, Pa) or equivalent.
- (b) Wrist-action shaker.—Burrell or equivalent.
- (c) Erlenmeyer flasks.—500 ml, ground-glass stoppered.
- (d) Chromatographic column.—Teflon stopcock, reservoir type (250 ml), 22 mm *O.d.* \times 300 mm *h.*
- (e) Funnel.—150 mm *d.*, with fluted filter paper to fit. Carl Schleicher & Schnell no. 588, or equivalent.
- (f) Hollow polyethylene stoppers.—Such as Nalgene's size 00.
- (g) Vials, 4 dram, screw cap with foil liners.—Kimble 60910-L.
- (h) Heating block, aluminum or brass. Drilled to accommodate vials.
- (i) Thin-layer chromatographic apparatus:
Glass plates, 20 \times 20 cm (8 \times 8"); Desaga-Brinkmann applicator or equivalent; mounting board; spotting template; microsyringe, 10 μ l; desiccating storage cabinet, Fisher 8-645-5 or equivalent; storage rack, Research Specialties Co., Richmond, California, or equivalent; Thomas-Mitchell tank; long-wave UV lamp, 15 W (use with ultraviolet-absorbing eyeglasses), or Chromato-Vue cabinet equipped with one or two 15-W lamps (Ultraviolet Products, Inc., San Gabriel, California 91776) or equivalent.

Reagents

- (a) Benzene, ACS grade.
- (b) Chloroform, ACS grade, n.b. specification on preservative, about 0.75 % EtOH.
- (c) Hexane, ACS grade.
- (d) Ether, diethyl, anhydrous, ACS grade.
- (e) Ethanol, ACS grade.
- (f) Methanol, ACS grade.
- (g) Sodium sulfate, anhydrous, ACS grade.
- (h) Silica gel for column chromatography, 0.05–0.20 mm; manufactured by E. Merck AG, Darmstadt, Germany. Activate by drying at 105 °C for 1 h, add 1 % H₂O by weight, seal, shake until thoroughly mixed, and store in air tight container 15 h before use.
- (i) Boiling chips.—SiC. Available from Carborundum Co., Niagara Falls, N.Y. 14303. Float off fines and extraneous matter with H₂O, wash with acetone, and dry.
- (j) Aflatoxin standards (see Appendix A).—Prepare solutions in benzene containing 0.5 µg B₁ and 0.5 µg G₁ per ml. Concentrations may be adjusted to suit analyst's perception sensitivity but the volume of the sample extract used in the preliminary TLC should be adjusted to obtain a comparable dilution factor.
- (k) Silica gel for thin-layer chromatography, G-HR.—Manufactured by Macherey, Nagel & Company, 516 Düren, Germany.
- (l) Glass wool.

Sample preparation

Peanut butters and peanut meals need no preparation for extraction unless they contain large particles, in which case some type of milling operation is necessary to reduce the particle size. Use a hammer mill, disc mill, or rotary cutter for meals. Grind samples of raw and roasted peanuts to a paste, using a disc (burr) type mill.

*Extraction**

Weigh 50 g sample (peanut butter, peanut meal, or finely ground peanuts) into a 500 ml glass stoppered Erlenmeyer flask. Add 25 ml distilled water and mix with a spatula until visually uniform. Add 250 ml chloroform and stopper. Shake one-half hour on a wrist-action shaker and filter through a fluted filter paper. Take 50 ml first portion chloroform filtrate.

*Column chromatography***

Place a ball of glass wool loosely in the bottom of a 22 × 300 mm chromatographic column and add approximately 5 g anhydrous sodium sulfate to give an even base for the silica gel. Add chloroform until the column is about

* Add 25 g Hyflo Super-Cel (Johns-Mauville Corp.) or equivalent to diatomaceous earth before shaking.

** Some laboratories have found that with extracts from low fat meals or defatted products the column chromatography can be dispensed with and thus shorten the procedure.

one-half full, then add 10 g silica gel (for column chromatography). Wash sides of column with about 20 ml chloroform, and stir to disperse silica gel in the chloroform. When rate of settling slows, draw off some of the chloroform to aid settling, leaving 2–3 inches of chloroform above the silica gel. Slowly add 15 g anhydrous sodium sulfate. Draw off the chloroform to the top of the sodium sulfate. Add the 50-ml sample extract (see previous paragraph) to the column and elute at maximum flow rate with 150 ml hexane followed by 150 ml anhydrous diethyl ether. Finally, elute the aflatoxin with 150 ml methanol/chloroform, 3/97, v/v. Collect the fraction from the time the methanol/chloroform was added until flow stops.

Add a few SiC boiling chips to the methanol/chloroform eluate, evaporate to near dryness on steam bath, and transfer residue quantitatively to vial with chloroform. Add 2–3 SiC boiling chips and evaporate chloroform, preferably under gentle stream of N_2 . Seal with hollow polyethylene stopper and cap. Save for thin-layer chromatography.

Thin-layer chromatography

Preparation of plates

Weigh 30 g silica gel G-HR into 300 ml stoppered Erlenmeyer flask, add approximately 60 ml H_2O , shake vigorously not longer than 1 minute, and pour into applicator. Adjust amount of water to obtain best consistency of slurry for spreading, as required by batch to batch variation in silica gel. Immediately coat 5 20 × 20 cm glass plates with 0.25 mm thickness of silica gel suspension, and let plates rest undisturbed until gelled (ca 10 minutes). Dry coated plates at least two hours at 80° and store in desiccating cabinet with active desiccant until just before use.

Preliminary thin-layer chromatography (TLC)

(This step may be omitted when approximate aflatoxin content is known.)

Uncap vial containing sample extract, add 500 μ l benzene, and reseal with polyethylene stopper. Shake vigorously to dissolve residue in benzene; use of a mechanical shaker is desirable. Puncture polyethylene stopper to accommodate needle of 10 μ l syringe. In subdued incandescent light, and as rapidly as possible, spot 1, 2.5, and 5 μ l on imaginary line 4 cm from bottom edge of TLC plate. Reseal and hold vial for quantitative analysis. On same plate spot 2, 5, and 10 μ l standard aflatoxins. At least one origin spot should contain all four aflatoxins to show whether adequate resolution is attained.

Place 50 ml of 1/9, v/v, acetone chloroform in the trough of an unlined developing tank. Immediately insert plate into tank (position plate to expose coated surface to maximum tank volume) and seal.

Develop plate for 40 min at 23–25 °C. Adjust development time to compensate if a different developing temperature is used. Remove from tank, let solvent evaporate and illuminate plate from below by placing it flat, coated side up, on long-wave ultraviolet lamp in darkened room. Alternatively, view plate in Chromato-Vue cabinet or illuminated from above. (If illumination requires looking directly at lamps, protect eyes with ultraviolet absorbing filter, such as Eastman 2A.) Observe pattern of 4 fluorescent spots of qualitative standard. In order of decreasing R_f they are B_1 , B_2 , G_1 , and G_2 . Note small color difference, bluish fluorescence of “B” contrasted with slightly green “G” aflatoxins. Examine patterns from sample for fluorescent spots having R_f close to, and appearances similar to those of standards. From this preliminary plate estimate suitable dilution for quantitative TLC analysis. In final calculations, take into account quantity of extract used for preliminary TLC.

Quantitative thin-layer chromatography

If, according to preliminary plate, a new concentration of sample extract is required, evaporate to dryness on steam bath and redissolve in estimated volume of benzene.

Spot successively 3.5, 5.0 and two 6.5 μ l portions of sample extract. All spots should be about the same size and not >0.5 cm. On same plate spot 3.5, 5.0, and 6.5 μ l of aflatoxin standards corresponding to those aflatoxins observed on the preliminary plate. Spot 5 μ l of each standard used on top of one of the two 6.5 μ l sample origin spots as an internal standard. Except for the revised volumes noted above, proceed as in preliminary thin-layer chromatography. At least one origin spot should contain all 4 aflatoxins to show whether adequate resolution is attained.

Interpretation of the chromatogram

4 clearly identifiable spots should be visible in the qualitative standard. If not, repeat chromatography, correcting or adjusting conditions to obtain proper resolution.

Examine pattern from sample spot containing internal standard for aflatoxin B₁ and G₁ spots. R_f values of B₁ and G₁ used as internal standards should be the same as, or should differ only very slightly from those of respective standard aflatoxin spots. (Since spots from sample extract are compared directly with standard aflatoxins on same plate, magnitude of R_f is unimportant. These may vary from plate to plate.)

Compare sample pattern with that containing internal standard. Fluorescent spots in sample thought to be B₁ or G₁ must have R_f values identical to and color similar to B₁ and G₁ only when unknown spot and internal standard spot are superimposed. Spot from sample and internal standard combined should be more intense than either sample or standard alone. Compare sample pattern with qualitative standard to determine if B₂ and G₂ are present.

Compare fluorescent intensities of B₁ spots of sample with those of standard spots and determine which of sample portions matches one of standards. To aid in the determination, ultraviolet light may be attenuated by moving plate away from lamp so that any particular pair of spots can be compared at extinction. Interpolate, if sample spot intensity is found to be between those of two of standard spots. If spots of smallest portion of sample are too intense to match standards, dilute sample and rechromatograph. Compare G₁ spots in same manner.

Assume that B₁ and B₂ have the same fluorescent intensity to weight relationships and compare B₂ spots of sample with B₁ standard spots to make quantitative estimate of B₂. Likewise, assume G₂ has same fluorescence intensity to weight relationship as G₁ and compare G₂ spot of sample with G₁ spot of standard.

Calculate concentration of aflatoxin B₁ in μ g/kg from formula: μ g/kg = $(S \times Y \times V)/(X \times W)$; where S = μ l of aflatoxin B₁ standard equal to unknown; Y = concentration of aflatoxin B₁ standard, μ g/ml; V = volume in μ l of final dilution of sample extract; X = μ l of sample extract spotted giving fluorescent intensity equal to S , the B₁ standard; W = grams of sample applied to column, 10 g if 50 ml chloroform extract is used. If final extract dilution does not represent 10 g, calculate correct sample weight and substitute. The 50-ml aliquot of the chloroform extract of a peanut butter or whole nuts removed for analysis usually contains 5–6 ml of fat which adds to the volume. Thus a 45-ml aliquot of chloroform has been removed and the

extract actually represents 9 g of starting material instead of the 10 g as for low fat materials.

Calculate aflatoxin G_1 in like manner.

Calculate B_2 and report as “ $\mu\text{g } B_2/\text{kg}$ based on fluorescence of B_1 ”.

Calculate G_2 and report as “ $\mu\text{g } G_2/\text{kg}$ based on fluorescence of G_1 ”.

Thin-layer chromatographic confirmation of aflatoxin G_1 and/or G_2

Confirm amount and identity of G_1 and G_2 by chromatography, using following solvent system:

Shake 46:35:19 (by volume) benzene:alcohol:H₂O in a separatory funnel. Let mixture stand overnight at room temperature (not $>22^\circ$). Carefully separate upper and lower phases.

Respot sample and standards on silica gel plate as in Quantitative TLC. Put 50 ml of lower phase in bottom of insulated, unlined developing tank. Put 50 ml of upper phase in trough. Without equilibrating, insert chromatoplate in trough (position plate to expose coated surface to maximum tank volume), and seal. Let solvent rise to stop line 12–14 cm above origin (30–50 min) and remove plate. In order of decreasing R_f values, qualitative standard gives B_1 , B_2 , G_1 , G_2 as before, but many extraneous fluorescent substances found in samples will have completely different R_f relative to those of aflatoxins in the 2 solvent systems. G_1 and G_2 aflatoxins of sample should have same R_f as those of respective standards. Make quantitative estimate for G_1 and G_2 as above.

Alternative thin-layer chromatography

Preparation of plates—same as above.

Initial thin-layer chromatography

Transfer residue in vial from column chromatography to small conical flask with 50 ml of chloroform.

Take a prepared TLC plate and score the coating with lines drawn approximately 0.5 cm in from each side edge. Draw a further line across the plate, parallel to the top edge and 4 cm from that edge to act as a solvent-front marker.

Along a line, which should not be marked on the coating, about 4 cm from the bottom edge of the plate spot out successively, in subdued light and as rapidly as possible, 5, 7.5, 10, 12.5, 15, 17.5, 20 and 22 μl of the chloroform filtrate, using a suitable micro-pipette. All spots should be of approximately the same area and should not exceed 0.5 cm in diameter. The larger volumes will have to be spotted on to the plate in several smaller portions.

Load at each side of the chromatoplate 5 μl portions of a qualitative standard containing all 4 aflatoxins.

Spots should be evenly spaced across the plate about 1.5 to 2 cm apart. (Up to twelve spots can be loaded on to one plate, if the spacing is kept to 1.5 cm.)

Immediately place the plate in a lined, equilibrated tank containing anhydrous diethyl ether (to a depth of about 2 cm), replace the lid and leave until the ether-front reaches the marked line. Take the plate from the tank and remove the ether by leaving at room temperature for a few minutes.

Fill a fresh unlined tank to a depth of about 2 cm with developing solvent (1:9, v/v, acetone : chloroform). Immediately stand the plate in the tank and replace the lid. Allow the plate to remain in the tank, at room temperature, until the solvent front reaches the marker line. Remove the plate from

the tank and allow all the developing solvent to evaporate before examining the plate under ultraviolet light.

(*Note:* The aflatoxins are sensitive to light, oxygen, acids and bases and many decompose if the plate is not developed immediately after spotting.)

Discard the developing solvent left in the tank.

Examination of developed plate

Place the plate face upward and irradiate with a long wavelength (365 m μ) ultraviolet lamp (Philips HPW 125 W bulb in a suitable starter unit) at a distance of 30 cm. Using two pieces of non-fluorescent matte black paper (film backing paper is suitable) blank off each spot and view separately; note the visibly fluorescent spots and their respective loadings for each of the aflatoxins B₁, B₂, G₁, and G₂ (the R_f values of these spots correspond to those of the four spots in the qualitative standard).

The estimation of the levels of the aflatoxins in the samples is based on the determination for each of the metabolites B₁, B₂, G₁, and G₂, of the minimum volume of extract which, when spotted onto a plate, developed and observed under ultraviolet light under standard conditions, produces a fluorescent spot which is *just* visible. The following procedure should be carried out for each of the four metabolites. For simplicity of wording, only one metabolite is considered in the description of the method, but it will be obvious that observations of fluorescence can be made on the spots of each of the metabolites at each dilution or concentration stage.

Quantitative examination

Observation of the first plate will provide one of the following conditions:

Spots are visible at some levels of loading: Note the smallest volume of extract loaded onto the plate which produces a spot with *just* visible fluorescence. If this spot results from a loading of less than 15 μ l, dilute the remainder of the extract such that, on repeating the procedure described above, the *just* visible fluorescence is seen in a spot resulting from a loading of 15 μ l or more. Record the volume loaded (S μ l) which produces just visible fluorescence, and the final volume (V ml) of the first aliquot of extract used. (If further dilution was unnecessary this will be 50 ml.)

Spots are visible at all levels of loading: In this case dilution of the extract is necessary. The following procedure is proposed as a guide but some may prefer to use intermediate dilution stages.

Dilute 25 ml of the extract to 100 ml with chloroform.

Repeat the chromatographic stage described above and observe the fluorescences of the spots produced. If some, but not all, are visible, proceed as described above.

If all the spots are visible, dilute 25 ml of the last solution used for spotting to 100 ml with chloroform, and repeat the procedure as before.

Repeat the dilution, if necessary, until the required visibility limit is reached.

Spots are visible at no levels of loading: In this case, concentration of the first aliquot is necessary. The following procedure is proposed as a guide, but some collaborators may prefer to use intermediate concentration stages.

Add 2-3 boiling chips to the flask and evaporate just to dryness, preferably under a gentle stream of nitrogen. Dissolve the residue in 5.0 ml chloroform, spot out portions, and proceed as described at the beginning of this alternative TLC procedure. If none of the spots are visible, remove

the solvent as before and dissolve the residue in 1.0 ml chloroform. If at this stage none of the spots are visible report the same as containing "Less than X $\mu\text{g/kg}$ ", where $X = F \times 10^6/112.5$ (for the definition of " F " see below).

Calculation of aflatoxin content of the sample

The aflatoxin content of the sample is calculated from the formula $\mu\text{g/kg} = (V \times F) 10^6/5S$, where:

V = volume (ml) to which the original aliquot of chloroform extract has been diluted or concentrated. (This volume is equivalent to the extract from 5 g of the sample. If no dilution or concentration of the original extract was necessary, then $V = 25$.)

S = volume (μl) loaded that gives a spot with a fluorescence which is *just* visible on the developed chromatoplate. (If the procedure suggested above is followed, then S will have a value of 15, 17.5, or 22.5.)

F = the smallest weight of aflatoxin (μg) which produces a spot with *just* visible fluorescence on the developed chromatoplate under the collaborators, standard conditions of illumination and viewing. If the conditions described above are used, then the values for F are: Aflatoxin B_1 and B_2 , 0.00036 μg ; Aflatoxin B_2 and G_2 , 0.00032 μg .

If the conditions for viewing the developed chromatoplate differ in any detail from those specified above, determine the appropriate values of F for these conditions. For this purpose suitable dilutions, in chloroform, of the quantitative standard should be used. (Assume that the value of F for aflatoxin G_2 is the same as that for aflatoxin B_1 ; similarly, the value for aflatoxin G_1 is the same as for aflatoxin G_2 .)

As a guide, it is suggested that the standard solutions be adjusted to a concentration of 0.02 $\mu\text{g/ml}$. These solutions, when spotted at the volumes given in the second paragraph of this alternative TLC procedure, will give an estimate of values of F . Using these first approximate values, further experiments may be carried out, at different loadings or dilutions, to obtain more precise values of F .

Appendix A

PROCEDURE FOR DETERMINATION OF AFATOXIN CONCENTRATION AND PURITY (including calibration of measuring instrument)

(I) *Aflatoxin Standards* may be obtained from :

Oilseed Crops Laboratory, US Department of Agriculture, Agricultural Research Service, PO Box 19687, New Orleans, La 70119 (USA)

or

Head, Department of Oil and Fat Research, Rijks Institute Voor de Volksgezondheid, Sterrenbos 1, Utrecht (Netherlands)

(II) *Calibration of instrument*

The instrument is calibrated with the same set of cells which will be used for the aflatoxin solutions.

(1) Dissolve 1.0 ml concentrated sulfuric acid (96%, sp.g. = 1.86) in 2.0 l distilled water to make a solution of approximately 0.018 N.

(2) Weigh accurately approximately 125 mg $K_2Cr_2O_7$ (Primary Standards) and dissolve in 1.0 liter 0.018 N H_2SO_4 . Calculate the molarity to three significant figures (Formula Weight of $K_2Cr_2O_7$ = 294.2). This solution should be approximately 0.4 mm.

(3) Make two accurate successive half dilutions of the acid dichromate solution from step 2 to prepare solutions of approximately 0.2 mm and 0.1 mm. Dilute with the 0.018 N H_2SO_4 .

(4) Determine the absorbance (A) of the three solutions (0.4 mm, 0.2 mm, 0.1 mm) at the wavelength of maximum absorption close to 350 m μ . Use the 0.018 N H_2SO_4 solution as the solvent blank in each case.

(5) Calculate the absorptivity (ϵ) at each of the concentrations by applying the equation:

$$\epsilon = \frac{(A) \times 1000}{\text{Concentration in mm}}$$

(6) If the three values vary by more than the guaranteed accuracy of the absorbance scale, check either the technique or the instrument. Average the three ϵ values from step 5 to obtain $\bar{\epsilon}$.

(7) Determine the correction factor (CF) for the particular instrument and cells in use by substituting into the equation:

$$CF = \frac{3,160}{\bar{\epsilon}}$$

If CF is <0.95 or >1.05, check either the technique or the instrument.

(III) *Determination of aflatoxin B₁ purity and concentration*

(1) Dependent on the TLC procedure selected, add benzene or chloroform (ACS grade) accurately to the container to give an estimated concentration of 10 μ g/ml. When benzene is the solvent, agitate vigorously to insure complete solution; use of a mechanical shaker is desirable.

(2) Determine the UV spectrum of this solution in the region 320–390 mμ. Use the same solvent in the reference cell as is used to dissolve the standard.

(3) Calculate the concentration of the aflatoxin solution by measuring the absorbance (A) at the wavelength of maximum absorption close to 350 mμ and applying the equation:

$$\text{Concentration } (\mu\text{g/ml}) = \frac{(A) (312) (1000) (CF)}{\epsilon}$$

Where (CF) is the correction factor obtained in step I (7) above, 312 = MW of aflatoxin B₁, and ϵ is absorptivity of aflatoxin B₁ at wavelength of maximum absorption. In benzene ϵ = 20,700; in chloroform ϵ = 21,800.

(IV) *Determination of aflatoxin G₁ purity and concentration*

(1) Dependent on the TLC procedure selected, add benzene or chloroform accurately to the container to give an estimated concentration of 10 μg/ml.

(2) Determine the UV spectrum of this solution in the region 320–390 mμ. Use the same solvent in the reference cell as is used to dissolve the standard.

(3) Calculate the concentration of the aflatoxin solution by measuring the absorbance (A) at the wavelength of maximum absorption close to 350 mμ and applying the equation:

$$\text{Concentration } (\mu\text{g/ml}) = \frac{(A) (328) (1000) (CF)}{\epsilon}$$

Where (CF) is the correction factor obtained in step I (7) above, 328 = MW of aflatoxin G₁, and ϵ is absorptivity of aflatoxin G₁ at the wavelength of maximum absorption; in benzene ϵ = 15,700; in chloroform ϵ = 17,600.

(V) *Determination of chromatographic purity*

(1) Follow first alternative thin-layer chromatography detailed in the assay procedure, except that the benzene/ethanol/water (confirmatory aflatoxin G system) developing system will be the only one employed.

(2) Spot successively at 2 cm intervals: the qualitative standard, 5 μl of aflatoxin B₁ (10 μg/ml), 5 μl of aflatoxin B₁ plus qualitative standard, 5 μl of aflatoxin G₁ (10 μg/ml), 5 μl aflatoxin G₁ plus qualitative standard, qualitative standard.

(3) The spots containing qualitative standards are for the determination of resolution effectiveness. The spots of B₁ and G₁ alone should reveal no other aflatoxins and only a faint display of fluorescent spots near the origin.

September, 1967

COLLABORATIVE STUDY OF "A VERSATILE PROCEDURE FOR ASSAY OF AFLATOXINS IN PEANUT PRODUCTS"*

By: R.M. EPPLEY, L. STOLOFF, and A.D. CAMPBELL (Division of Food Chemistry, Food and Drug Administration, US Department of Health, Education and Welfare, Washington, DC 20204)

Abstract

A collaborative study of the CB procedure for aflatoxin in peanut products was carried out with naturally contaminated peanut butter and peanut meal and aflatoxin-free butter to which known amounts of aflatoxin B₁ and G₁ were added. Part of the study included preparatory isolation of the aflatoxin B₁ found in the naturally contaminated samples and confirmation of the identity by both chemical and biological tests.

The results from 13 collaborators demonstrate both between and within laboratory precision equal to, and accuracy probably better than the official, first action procedure; advantages in speed and convenience were noted. The preparatory separation was easily accomplished with clear chemical and biological proof of satisfactory isolation by 7 of the 9 participants in this phase of the study.

The "versatile procedure for assay of aflatoxin in peanut products" [1] is considered to be a rapid and sensitive method. Initial studies indicated that the CB procedure is at least as accurate and sensitive as the official, first action procedure [2] which has been thoroughly tested [3, 4]. Sample sizes are conveniently adjusted from a single kernel to a kilogram or more for isolation of sufficient aflatoxin for confirmation tests by bioassay [5] or chemical derivative [6, 7].

A collaborative study of the CB procedure was carried out with naturally contaminated peanut butter and peanut meal and aflatoxin-free butter to which known amounts of aflatoxins B₁ and G₁ were added (spiked samples). Part of the study included preparatory isolation of the aflatoxin B₁ found in the naturally contaminated samples and confirmation of the identity by both chemical and biological tests.

Description of samples

The peanut butters were thoroughly blended and 50-g portions weighed into 4-oz glass jars. For the spiked samples, the aflatoxins were metered by pipette from chloroform solution directly into the individual jars containing the aflatoxin-free peanut butter. The collaborators were directed to use the entire contents of each jar for analysis.

Each collaborator was provided with 8 samples as outlined in Table I. 9 of the 13 collaborators were each provided with 1 kg of the naturally contaminated peanut butter and of the peanut meal.

Description of study

Each collaborator was sent the 8 randomly coded samples, quantitative standards of aflatoxin B₁, B₂, G₁ and G₂, instructions, reporting forms, and a copy of the method.

The 9 laboratories that received the kilogram samples of peanut butter and peanut meal were directed to analyze 50-g portions for all 4 aflatoxins.

* Published in JAOAC 51, 67-73; 1968, slightly modified in several instances.

From the calculated amounts in the sample determine the quantity of sample containing 50 μg of aflatoxin B_1 , then process this amount by the CB preparatory procedure to provide extract for use in the identification procedures [5, 7] and for confirmation of the original quantitative estimations. The preparation of chromatographically pure aflatoxin B_1 as described for the chemical confirmation [7] tests was scaled up to include the quantity required for toxicity tests [5]. The starting amount of aflatoxin B_1 was based on an estimated 50% recovery from the chromatographic procedures. To check this recovery, data on the measured amounts of aflatoxin B_1 in the extract before and after preparatory TLC were requested.

The analysts were directed to remove 1 μg of the recovered B_1 for chemical derivative identification [7], 10–15 μg for chick embryo assay [5] and to hold the remainder for an anticipated brine shrimp bioassay [8]. They were also instructed to prepare a photograph of the chemical derivative TLC plate for inclusion with the final report. The 4 laboratories that did not participate in the preparatory scale phase of the study were supplied with 50 g of each of the naturally contaminated material, randomly coded, to be handled in the same manner as the spiked samples.

The quantitation part of this study was designed to measure accuracy and precision between and within laboratories. The remainder of the study was to determine laboratory capability for complete follow through on the identification and confirmation of aflatoxin in naturally contaminated samples.

Method

Apparatus

- (a) Disc mill.—Model 4E, Straub Co. (Quaker City Grinding Mills, Philadelphia, Pa), or equivalent.
- (b) Wrist-action shaker.—Burrell or equivalent; or stirring motor 1/30 hp, 1400–1600 rev/min, equipped with stainless steel shaft and propeller blade.
- (c) Erlenmeyer flasks.—500 ml, ground-glass stoppered.
- (d) Rotary evaporator with continuous feed.
- (e) Chromatographic column.—22 \times 300 mm with Teflon stopcock, reservoir type (250 ml); or 45 \times 600 mm.
- (f) 12 qt stainless steel pail.
- (g) Funnel.—150 ml with fluted filter paper to fit; or Buchner funnel, 32 cm diameter, with Whatman No. 1 or equivalent filter paper to fit.
- (h) Vials.—4 dram, foil-lined screw-cap, Kimble 609010-1.
- (i) Hollow polyethylene stoppers.—Such as Nalgene's size 00.

Reagents

- (a) Solvents.—ACS grade; benzene, chloroform, hexane, anhydrous diethyl ether, and methanol.
- (b) Sodium sulfate.—Anhydrous, ACS grade.
- (c) Silica gel.—For chromatography: 0.05–0.2 mm (for 50 g sample) or 0.2–0.5 mm (for 1-kg sample); Brinkmann Instruments, Inc., Westbury, NY. Activate by drying at 105 $^{\circ}\text{C}$ for 1 h, add 1% H_2O by weight, seal, shake until thoroughly mixed, and store in air-tight container.
- (d) Diatomaceous earth filter-aid.—Celite, Hyflo Super-Cel (Johns-Manville Corp.), or equivalent.
- (e) Boiling chips.—SiC. Available from Carborundum Co., Niagara Falls, NY 14303. Float off fines and extraneous matter with H_2O , wash with acetone, and dry.
- (f) Aflatoxin standards.—Prepare solutions in benzene containing 0.5 μg B_1 , 0.25 μg B_2 , 0.5 μg G_1 , and 0.25 μg G_2 per ml. The standard solutions can

be prepared separately or in any combinations desired. Concentrations may be adjusted to suit analyst's perception sensitivity, but the volume of the sample extract used in the preliminary TLC should be adjusted to obtain a comparable dilution factor.

(g) Silica Gel G-HR. — Brinkmann Instruments, Inc., Westbury, NY 11590.

(h) Glass wool.

Sample preparation

Peanut butters and peanut meals need no preparation for extraction unless they contain large particles, in which case some type of milling operation should be used to reduce the particle size. Use a hammer mill or rotary cutter for meals. Samples of raw and roasted peanuts must be ground to a paste before extraction. For this operation and for "chunky-type" peanut butter use a disk (burr) type mill.

Extraction

50-g samples. — Weigh sample into a 500-ml glass-stoppered Erlenmeyer flask. Add 25 ml distilled water, 25 g of diatomaceous earth, 250 ml CHCl_3 and tape a stopper in place. Shake for 30 min on a wrist action shaker and filter through a fluted filter paper. If filtration is slow or difficult, transfer to a Buchner funnel and use light vacuum. Vacuum filtration is only recommended for the slow filtering samples since evaporation of the chloroform is rapid under vacuum, resulting in concentrating of the extract.

Collect the first 50-ml portion of the CHCl_3 filtrate and proceed to the silica gel column cleanup step.

1-kg sample. — Weigh the finely divided material into a 12 qt stainless steel pail. Add 500 ml distilled water, 5 l CHCl_3 and cover the pail, leaving a small opening for the stirrer shaft. Position the stirrer to achieve maximum agitation without splashing. Stir for 30 min, mix in 500 g filter-acid, and immediately filter through Buchner funnel.

Remove a 50-ml portion of the CHCl_3 filtrate for check analysis, starting with *column chromatography* for the 50-g sample. Wash the solids on the funnel with 1 l CHCl_3 and concentrate the combined CHCl_3 filtrates in the rotary evaporator to a small volume—ca 800 ml when the sample contains fat and ca 200 ml for low fat meals. Add 1 l hexane/ CHCl_3 (1/1, v/v) to the concentrated extract and proceed to the silica gel column cleanup step.

With some samples a precipitate may appear in the sample/hexane/chloroform mixture which could cause the silica gel column to plug. If a precipitate appears, filter the extract through a bed of filter-aid in a Buchner funnel, washing the solid with 1000 ml of CHCl_3 hexane 1/1, v/v.

Column chromatography

50-g sample. — Place a ball of glass wool loosely in the bottom of a 22 × 300 mm chromatographic column and add ca 5 g anhydrous Na_2SO_4 to give an even base for the silica gel. Add CHCl_3 until the column is about one-half full; then add 10 g silica gel (0.05–0.2 mm). Wash sides of column with about 20 ml chloroform, and stir to disperse silica gel in the chloroform. When rate of settling slows, draw off some of the chloroform to aid settling, leaving 2–3 in. of chloroform above the silica gel. Slowly add 15 g of anhydrous sodium sulfate. Draw off the chloroform to the top of the sodium sulfate. Add the 50 ml of sample extract to the column and elute at maximum flow rate with 150 ml of hexane followed by 150 ml of anhydrous diethyl ether. Finally, elute the aflatoxin with 150 ml of methanol/chloroform, 3/97, v/v. Collect the fraction from the time the methanol/chloroform was added until flow stops.

Add a few SiC boiling chips to the methanol/chloroform eluate, evaporate to near dryness on steam bath, and transfer residue quantitatively to vial with CHCl_3 . Add 2-3 SiC boiling chips and evaporate CHCl_3 , preferably under gentle stream of N_2 . Seal with hollow polyethylene stopper and cap. Save for thin layer chromatography.

1-kg sample.—Prepare the column as above, using a 45×600 mm chromatographic column, 20 g Na_2SO_4 on the glass wool ball, 100 g silica gel (0.2-0.5 mm), and 150 g Na_2SO_4 on top of the silica gel. Elute at 40-60 ml/min, follow with 500 ml CHCl_3 /hexane (1/1, v/v), 1.5 l anhydrous diethyl ether, and 1 l methanol/ CHCl_3 (3/97, v/v).

Add a few SiC boiling chips to the methanol/chloroform eluate and evaporate to dryness on a steam bath or a rotary vacuum evaporator. Transfer the residue quantitatively to a vial with CHCl_3 , add 2-3 SiC boiling chips and evaporate the CHCl_3 , preferably under a gentle stream of N_2 . Seal with a hollow polyethylene stopper and cap. Retain extract for quantitation and/or preparatory separation of aflatoxin B_1 as described in "Changes in methods" [7].

Thin-layer chromatography and calculations

The thin-layer chromatography (TLC) analysis and calculations (except as noted below) are performed as described in the "Changes in methods" [1], substituting acetone/chloroform (1/9, v/v) in an unlined and unequilibrated tank as the developing system [10].

The 50-ml aliquot of the chloroform extract of peanut butter or of whole nuts removed for analysis usually contains 5-6 ml of fat, which adds to the volume. Thus a 45-ml aliquot of chloroform has been removed and the extract actually represents approximately 9 g of starting material, instead of the 10 g as for low fat materials.

Results and discussion

The analytical results reported by the individual collaborators are presented in Table I. 4 of the 13 collaborators reported the presence of small amounts of both aflatoxins B_1 and G_1 in the blank sample. Extraneous fluorescents from peanuts are at times falsely reported as low levels of aflatoxins. These false positive reports were disregarded in the statistical analysis. On the basis of the "Youden Rank Sum Test" [9], the results of collaborator No.4 for the samples with added aflatoxins were discarded as "outliers".

The average percent recoveries decreased with increasing concentrations for both aflatoxin B_1 and G_1 . This indicates a contributing effect of extract components as the ratio of background to aflatoxin increases. CAMPBELL and FUNKHOUSER [4] reported in their collaborative study of the official, first action procedure, a similar trend:

Aflatoxin B_1 added $\mu\text{g/kg}$ sample	Aflatoxin B_1 reported % of added
10	121
30	88
40	79
50	72
110	72

Since no spiked samples above 45 $\mu\text{g/kg}$ were included in this study, we can only speculate whether recoveries would have continued to decrease or remain at approximately 100%.

As a means of between laboratory precision, the average coefficient of variation was computed from the between laboratory standard deviations for the aflatoxin B₁ assays. A similar computation was made from the standard deviations reported from the collaborative study of the official, first action procedure [4]. Data from pairs in that study were used to compute the average within laboratory coefficient of variation for aflatoxin B₁ assays, and the triplicate set in the present study was used for the same purpose. Data from samples at a level of 10 µg/kg were excluded as obviously outside the quantitative limits of both procedures.

Although the average coefficients are not strictly comparable because of differences in experimental structure, the gross comparison (Table II) indicates a similarity of precision between and within laboratories and between the 2 procedures.

Resolution of the 4 aflatoxins from each other on the TLC plate offered no difficulty using the acetone/chloroform developing system [10], but interference in the aflatoxin G area of the TLC plates was reported by 8 of the 13 collaborators for extracts from the spiked samples. This interference consisted of a streak on the TLC plate extending from the origin to the *R_f* area of the aflatoxin G's. The aflatoxin G's in the sample extracts (internal standards) were pushed to a higher *R_f* than the external standard spots. This problem was traced to a component of the peanut butter, which may have developed on storage, since this interference has not been observed with fresh samples. The peanut butter used in this study was from a "clean" stock obtained several years ago and held in 4° storage. The interference difficulty probably accounts for the poor precision in the quantitation of aflatoxin G₁ and the frequent reporting of significant quantities of aflatoxin G₁, where none had been added. None of the collaborators used the alternative developer (benzene/ethanol/water) to confirm the identity of the aflatoxin G's, as detailed in the directions. This portion of the instructions may need stronger emphasis.

The collaborators' comments described the method as easy to perform, rapid, and yielding clean extracts for TLC, except for the interference from the peanut butter extract in the G area of the spiked sample chromatographs.

Several minor changes resulting from collaborator comments and additional information obtained after completion of the study have been incorporated into the procedure. Diatomaceous earth was found to give better filtration and somewhat cleaner final extracts when present during extraction without having any effect on recoveries. Premixing of the water with the sample was found to be an unnecessary labor, since the shaking of the extraction process proved to be adequate to insure its incorporation in the solid phase. Benzene instead of chloroform is preferred as a solvent for the standards and the final spotting extract. This has been covered in a separate report [11]. All these changes are included in the foregoing description of the procedure, even though not part of the collaborative study.

Preparatory Procedure and Confirmation of Identity

9 laboratories collaborated in this phase of the study. Reported recoveries and confirmation of the identity of the recovered products are given in Table IV. Positive chemical derivatives were reported by all laboratories. 7 laboratories submitted photographs of the identifying TLC plates from which the identifications were corroborated, except for 5 questionable acetic acid reaction products. The photographic evidence indicated possible difficulty in maintaining anhydrous conditions required for this reaction [6].

The chick embryo bioassay* [5] was performed at dosage levels indicated by the reported recovery of aflatoxin B₁. The assays were rerun at increased levels when necessary to obtain a positive response.

Positive responses were obtained from 14 of the 18 presumed isolates of aflatoxin B₁, 11 at 1X, 1 at 1.5X, 1 at 2X, and 1 at 4X the expected lethal dosage from the amounts reported. No biological activity was seen with 3 of the isolates, 1 at 4X and the other 2 at 8X the expected lethal dosage. A questionable response was obtained with a reported 3 µg of isolates, too little for a good test. The 2 isolates giving negative bioassays at 8X, the expected lethal dose, were from one laboratory, which reported 100 percent recoveries an unrealistic figure. The photographs of the chemical derivative confirmation from this laboratory showed expected reaction products, but the recovery data must be incorrect by more than a factor of 8 for the observed negative bioassay. The positive bioassay at 4X the expected dosage was from an estimated 93 percent recovery, which if corrected by this factor, is in better agreement with the recovery and assay data from the same laboratory (No. 8) for the isolate from its other sample. One negative bioassay result at 4X anticipated dose has no explanation.

Table IV shows a comparison of the analytical results obtained from the 50-g CB procedure and the CB preparatory procedure for the naturally contaminated samples. None of the results from the 9 collaborators were excluded from these calculations. The standard deviations and coefficient of variations are remarkably consistent for the two procedures considering the differences in sample size and operations. Some bias may be present in the determination of the quantities present in the preparatory procedure extract, since the operator has on hand the results for the 50-g sample. From the coefficients of variation it is evident that these samples were homogeneous throughout, since there is no significant difference between coefficients for the 2 sample sizes.

No serious criticism of the procedure or description was received. The preparatory procedure has been presented on the basis of a 1-kg sample. Adjustments to other size samples are easily made by using the appropriate ratios of solvents and equipment. The same size preparatory silica gel column should be used regardless of sample size.

Conclusions

The results of this study show that compared to the official, first action procedure for aflatoxins in peanut products, the CB procedure is possibly more accurate, as judged from recovery data, and equal in precision. Decreased elapsed time and operator time, and simplicity of required equipment are advantages.

The effectiveness and simplicity of the scaled-up procedure for preparatory isolation of presumptive aflatoxins for confirmatory tests were amply demonstrated.

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Table 1 Analytical results reported by individual collaborators—Aflatoxins, $\mu\text{g/kg}$ sample

Sample	1	2						3			4-5-6		7		8									
		Peanut butter						Peanut meal			Natural		Natural											
Product		Added		Added		Added		Added		Added		Natural		Natural										
Aflatoxin source	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-							
Aflatoxin amount, µg/kg	0	0	0	10	0	0	20	10	35	45	57	58	57	57	0	0	0	0						
Aflatoxin identity	B ₁	G ₁	B ₁	G ₁	B ₁	G ₁	B ₁	G ₁	G ₁	B ₁	B ₁	B ₁	B ₁	B ₁	B ₁	B ₁	B ₁	B ₁	G ₁	G ₂				
Laboratory																								
1	0	0	0	14	0	0	28	0	0	57	58	57	57	57	0	0	85	60	192	135	0	0		
2	0	0	0	11	0	0	22	3*	33	56	33	33	56	56	33	74	56	93	22	300	50	50	20	
3	0	0	0	22	0	0	22	11	44	44	56	44	44	44	33	44	33	111	11	250	25	3*	3*	
4†	0	0	0	0	0	0	10	0	0	0	0	0	55	55	0	0	55	56	11	100	13	13	?	
5	0	0	0	25	0	0	25	0	0	25	25	25	25	25	50	0	0	89	14	250	18	50	0	0
6	0	56	0	28	0	28	0	56	111	56	28	56	56	111	83	111	83	111	7	250	19	50	0	0
7	7	8	3*	8	0	0	16	3*	38	30	3*	30	38	20	33	38	38	115	18	201	20	28	14	14
8	0	0	0	0	0	0	30	0	0	30	110	10	0	0	0	0	0	28	8	90	18	0	0	0
9	3*	25	17	25	29	30	29	30	55	43	47	55	47	55	79	55	55	83	20	200	20	100	7	7
10	0	0	27	0	27	27	27	27	35	50	65	37	27	65	37	27	65	50	0	93	0	65	0	0
11	9	8	22	7	25	10	25	10	45	46	38	28	**	26	28	**	26	48	8	201	17	20	9	9
12	7	8	14	7	16	8	16	8	53	44	35	23	17	21	23	17	21	43	12	123	17	14	9	9
13	0	?	17	0	30	?	30	?	52	38	55	21	?	?	?	?	?	75	11	204	13	14	0	0
Average			14		23	13	23	13		44					36			78	16	196	29			
Range			0-27		0-30	0-56	0-30	0-56		0-110					0-111			28-115	0-60	90-300	0-135			
Standard deviation			±9		±8	±18	±8	±18		±17					±49			±29	±15	±65	±35			
Standard error			±3		±2	±5	±2	±5		±3					±5			±8	±4	±19	±10			
Coefficient of variation, %			64		35	139	35	139		39					136			37	94	33	121			

Could not be determined because of interference in G area

⊕ Omitted spiked samples from statistical calculations as outliers

*Reported as trace

****Sample lost**

Table II Average coefficients of variation for aflatoxin B₁ assays

Procedure	Between laboratories	Within laboratories
Official first action	30%	45%
CB	37%	38%

Table III Collaborator reports of aflatoxin B₁ recovery from preparatory separation and derivative identification of isolated product, compared with the chick embryo bioassay of the isolated products

Laboratory	Sample	Reported aflatoxin B ₁		Aflatoxin derivative with			Chick embryo bioassay	
		μg re-covered	Percent recovery	TFA ¹	F ²	AcH ³	Re-sponse	Dose* level
1	Butter	12/30	40	+	+	+	+	1 X
	Meal	15/39	38	+	+	+	—	4 X
2	Butter	22/50	44	+	+	+	+	1 X
	Meal	12/28	43	+	+	+	+	1 X
3	Butter	25/70	36	+	+	+	+	1 X
	Meal	15/50	30	+	+	+	+	1 X
4**	Butter	28/35	80	+	+	+	+	1 X
	Meal	23/35	66	+	+	+	+	1 X
5**	Butter	3/25	12	+	+	+	?	?
	Meal	7/25	21	+	+	+	+	2 X
6	Butter	35/35	100	+	+	±	?	8 X
	Meal	35/35	100	+	+	±	—	8 X
7	Butter	25/65	38	+	+	±	+	1 X
	Meal	25/65	38	+	+	±	+	1 X
8	Butter	10/50	20	+	+	±	+	1.5 X
	Meal	50/54	93	+	+	±	+	4 X
9	Butter	35/50	70	+	+	+	+	1 X
	Meal	35/50	70	+	+	+	+	1 X
		Average	47					

*Nominal level divided by level indicated by biological response

**Analysts reported positive derivatives but did not submit photographs for confirmation

? Questionable observations

± Borderline observations

Aflatoxin derivative (1) with trifluoroacetic acid (2) with formic acid and thionyl chloride (3) with glacial acetic acid and thionyl chloride

Table IV Analytical results reported by individual collaborators, comparison of sample size— aflatoxins, $\mu\text{g/kg}$

Sample	Peanut butter								Peanut meal							
Sample size	50 g				Preparatory				50 g				Preparatory			
Aflatoxin	B ₁	B ₂	G ₁	G ₂	B ₁	B ₂	G ₁	G ₂	B ₁	B ₂	G ₁	G ₂	B ₁	B ₂	G ₁	G ₂
Laboratory																
1	85	60	0	0	86	46	0	0	192	135	0	0	260	108	0	0
2	93	22	0	0	91	18	0	0	300	50	50	20	280	40	T	T
3	111	11	0	0	125	17	T*	T	250	25	T	T	167	17	T	T
4	56	11	0	0	50	8	0	0	100	13	13	—	86	13	13	—
5	89	14	0	0	83	11	0	0	250	18	50	10	208	17	29	11
6	111	7	0	0	144	18	0	0	250	19	50	0	232	15	20	0
7	115	18	8	4	108	Not estimated			201	20	28	14	217	Not estimated		
8	28	8	0	0	27	Not estimated			90	18	0	0	97	Not estimated		
9	83	20	36	0	72	9	41	0	200	20	100	7	150	13	5	5
Average	86	19			87	18			182	31			189	32		
Standard deviation	28	16			36	13			98	43			78	35		
Coeffic. of variation, %	33	84			42	72			54	139			41	109		
Range, hi	115	60			144	46			300	135			280	108		
lo	28	7			27	8			90	18			86	13		

T = Trace present

CALENDAR

* = not sponsored by IUPAC

1968

March 11-14	Symposium on Modern Chemistry in Industry	Eastbourne (UK)
March 14-16	Symposium on Standards for High Pressure Research	Gaithersburg, Maryland (USA)
April 1-5	Joint Annual Meetings	Dublin (Ireland)
March 31- April 5	CLVth National Meeting of the American Chemical Society	San Francisco Cal. (USA) *
April 8-10	IIIrd European Symposium: "Food—Recent Development in Food Preservation"	Bristol * (UK)
April 9-12	Konferenz über Apparate der chemischen Industrie	Budapest * (Hungary)
April 17-19	XIXe Congrès: "Journées de la Chimie 1968"	Milan * (Italy)
May 13-17	International Symposium on the Recovery of Pulping Chemicals	Helsinki (Finland)
May 16-17	General Assembly – la Société Chimique de France	Montpellier * (France)
June 17-21	Symposium on the Structure and Chemistry of Solid Surfaces	Berkeley Cal. (USA)
June 20-21	Dechema-Jahrestagung 1968	Frankfurt * (Germany)
June 23-29	IVth International Congress on Catalysis	Moscow (USSR)
July	IIInd International Symposium on the Chemistry of Organic Silicon Compounds	Bordeaux (France)
July 8-11	Symposium on Nuclear Magnetic Resonance	São Paulo * (Brazil)
July 8-13	Vth International Symposium on the Chemistry of Natural Products	London (UK)
July 22-26	2nd International Symposium "Pharmaceutical Chemistry" (see "Bulletin" 30, p. 43)	Münster (Germany)
August	VIth International Symposium on the Reactivity of Solids	Schenectady New York (USA)
September 2-6	IIIrd International Symposium on Fermentation	New Brunswick (USA)
September 3-6	Symposium on Properties of Macromolecular Systems	Toronto (Canada)
September 4-6	International Conference on Electrophotography (Dr. W. Lewis Hyde, Institute of Optics, University of Rochester, Rochester, NY, USA)	Rochester * (USA)
September 8-12	XIth International Conference on Coordination Chemistry	Haifa (Israel)
September 10-13	Analytical Chemistry Symposium	Warsaw (Poland)

September 10-13	Chemical Aspects of Paper Making	Praha (CS)
September	Symposium Valence Tautomerism	Karlsruhe (Germany)
September 16-18	XIth International Conference on Coordination Chemistry	Jerusalem (Israel)
1968 or later	Carbohydrate chemistry	Paris
	1969	
4th week in April	Symposium on Natural Products	Mexico
1st decade in July	XXVth International Conference of Pure and Applied Chemistry including a Symposium	Cortina d'Ampezzo (Italy)
July 10	International Symposium on Analytical Chemistry	Birmingham (UK)
3rd week in July	Symposium on Chemical Control of Human Environment	Johannesburg, Pretoria (South Africa)
July 14-18	IVth International Congress on Pharmacology	Basle * (Switzerland)
August 20-27	XXIInd International Congress of Pure and Applied Chemistry and XIIth International Conference on Coordination Chemistry	Sydney (Australia)
August 25-30	Symposium on Kinetics and Mechanism of Polyreaction (Macromolecular Division)	Budapest (Hungary)
To be decided	Symposium on Nonaqueous Electrochemistry	To be decided *
September 8-13	VIIth International Congress on Clinical Chemistry	Geneva (Switzerland)
1969 or 1970	Cyclo-Addition	Munich (Germany)
	1970	
	VIth International Symposium on Microchemistry	Graz (Austria)
	Symposium on the Chemistry on Natural Products organized by the Academy of Science of the USSR	Riga
	Symposium on Carbohydrate Chemistry sponsored by the Division of Organic Chemistry	
	Symposium on Macromolecular Physics (Macromolecular Division)	Leiden or Delft
	1971	
July	XXVth International Conference of Pure and Applied Chemistry	Wash. DC (USA)
	International Congress of Pure and Applied Chemistry	Boston Mass. (USA)
	Symposium on Macromolecular Chemistry	Boston Mass. (USA)

LIST OF ABBREVIATIONS

AOAC	Association of Official Agricultural Chemists
CBN	Commission on Biochemical Nomenclature
CEBJ	Commission of Editors of Biochemical Journals
CEE	Communauté Economique Européenne
CIG	Comité International de Géophysique
CIPM	Comité International de Poids et Mesures
CITCE	Comité International de Thermodynamique et Cinétique Electrochimique
CNRS	Centre national de la Recherche scientifique
COMECON	Council for Mutual Economic Assistance
COSPAR	Committee on Space Research
CSF	Compagnie Télégraphie Sans Fil
CSIRO	Commonwealth Scientific and Industrial Research Organization
DECHEMA	Deutsche Gesellschaft für chemisches Apparatewesen eV
EEC	European Economic Community
EMPA	Eidgenössische Materialprüfungs-Anstalt
EPPO	European and Mediterranean Plant Protection Organization
ETH	Eidgenössische Technische Hochschule (Zürich)
EUCEPA	European Committee on Cellulose and Paper
EUROTOX	Comité européen permanent pour la Protection des populations contre les risques de toxicité à long terme
FAGS	Fédération of Astronomical and Geophysical Services
FAO	Food and Agriculture Organization
GEFAP	Groupement européen des Associations nationales de Fabricants de Pesticides
IAEA	International Atomic Energy Agency
IAMS	International Association of Microbiological Societies
IAPT	International Association for Plant Taxonomy
IASH	International Association of Scientific Hydrology
IAU	International Astronomical Union
IBP	International Biological Programme
ICCA	International Commission for Cellulose Analysis
ICSU	International Council of Scientific Unions
ICUMSA	International Committee for the Unification of Methods of Sugar Analysis
IGU	International Geographical Union
IMU	International Mathematical Union
ISO	International Organization for Standardization
ITU	International Telecommunication Union
IUB	International Union of Biochemistry
IUBS	International Union of Biological Sciences
IUCr	International Union of Crystallography
IUGG	International Union of Geodesy and Geophysics
IUGS	International Union of Geological Sciences
IUNS	International Union of Nutritional Sciences
IUPAC	International Union of Pure and Applied Chemistry
IUPAP	International Union of Pure and Applied Physics
JCAM	Joint Commission on Atomic Masses
JCAR	Joint Commission on Applied Radioactivity
MIT	Massachusetts Institute of Technology
NAS	National Academy of Sciences

NATO	North Atlantic Treaty Organization
NBS	National Bureau of Standards
NRC	National Research Council
OECD	Organisation de Coopération et de Développement économiques
OEPP	Organisation européenne de Protection des Plantes
OMS	Organisation Mondiale de la Santé
SCAR	Scientific Committee on Antarctic Research
SCOR	Scientific Committee on Oceanic Research
UICC	Union internationale contre le Cancer
UNESCO	United Nations Educational Scientific and Cultural Organization
WHO	World Health Organization
WMO	World Meteorological Organization



**INTERNATIONAL UNION OF PURE
AND APPLIED CHEMISTRY**

**UNION INTERNATIONALE DE CHIMIE
PURE ET APPLIQUÉE**

50 YEARS IUPAC


1918–1968

**INFORMATION BULLETIN
NUMBER 32**

AUGUST 1968

SECRETARY GENERAL:

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Cable address: IUPACAIRPORT

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INTRODUCTION

The last Information Bulletin, No.31, dated March 1968, was compiled under great pressure of time and an overload of work. Nobody who has not seen the removal of the files from the office and archives can have any idea of the enormous detailed work involved: there were 50 boxes of some 80 lb each, 21 boxes were shipped to Oxford, 25 were sent to the Federal Institute of Technology in Zurich, 6 boxes are in storage with an international transport company, and finally the remainder came to the Zurich Secretariat. The archives from Paris have still not been touched. Now we are well established at the Zurich Airport and you have received from Dr MAURICE WILLIAMS, who has been appointed as Executive Secretary from 1 April, 1968, communication that his office in Oxford is functioning. His address is: 2-3 Pound Way, Cowley Centre, Oxford, U.K.

Bürgenstock Meeting on Stereochemistry

Thanks to the CIBA Foundation in London and co-sponsored by IUB and the International Union of Pure and Applied Chemistry, a symposium was held on Stereochemistry Nomenclature, to which representatives of all Nomenclature Divisions were invited. IUPAC specifically made it possible for A.M. SARGESON (Dept of Inorganic Chemistry, The Australian National University, Canberra), to attend this meeting.

Following this very important meeting, the traditional Scientific Conference on Stereochemistry was held on the Bürgenstock, Switzerland.

Thanks to the kindness of Prof. A. ESCHENMOSER (ETH), the Secretary General was invited to attend for two days, although the Bürgenstock meeting is no longer sponsored by IUPAC (it belongs to EUCHM Conferences). In view of the close connection with the aforementioned Symposium on Nomenclature, it seems necessary and well indicated to say here a few words about the Bürgenstock meetings:

The Bürgenstock meeting, right from the beginning, was concentrated, or if you prefer, limited to Stereochemistry. The selection of the distinguished people from the Zurich ETH and University has proved to be a capital idea, in both their choice of the topic Stereochemistry and the place, Bürgenstock. In order to demonstrate clearly the three dimensions in Stereochemistry, you need an environment which also shows the three dimensions very clearly. For that reason, Bürgenstock on the Lake of Lucerne, is an excellent choice, in spite of the fact that the Bürgenstock and the Bürgenstock Conference are on a "pretty high level". The mountains around the Lake of Lucerne vary in height between some 3000 and 7000 ft, Bürgenstock 3000 ft, Stanserhorn 6235 ft and Pilatus 6993 ft.

On the occasion of the last meeting held on the Bürgenstock, some participants even went as high as on the Titlis Mountain (10627 ft). It is well understood that also with regard to the scientific content of the deliberations, similar reflexions could be made. Concerning the rates of the Bürgenstock hotels, our friend FRITZ FREY chose his lowest level which was still "pretty high" in spite of the timing in the off-season.

The IUPAC Nomenclature Commissions may profit from the Bürgenstock meeting in ironing out their rules for Stereochemistry Nomenclature which will be in the next Information Bulletin. It is hoped that the blocks for the complicated formulae will be ready in time.

The location of the Secretariat General at the Zurich Airport is an excellent one and outweighs the drawback of our poor working conditions. The convenience of the situation at the Zurich Airport was unquestionably

proved recently at a meeting for coordination of the Analytical Methods and in a most striking way at the meeting of the Division Presidents. This meeting, urgently requested by the Executive Committee, had to be changed at the very last minute from Paris to Zurich, after consultation with our friends from the Royal Society in London. It is always extremely difficult to fix convenient dates for some 6 to 10 distinguished experts from many countries. The President of the Analytical Division, Prof. P. WEST, Bâton Rouge LA, received the cable on Tuesday and was able to arrive in Zurich as early as Wednesday midday. The first meeting was held, for the convenience of all persons present, in the Union Bank of Switzerland in Zurich and the second day's meeting took place right on top of the airport building, so that those Division Presidents who were under pressure of time, could stay at the meeting until 10 minutes before their departure by plane.

This Information Bulletin is the most voluminous one ever published, because the Joint IUB/IUPAC Nomenclature Commission is eager to distribute their proposals worldwide and without delay. Also, some reports of Divisions, Sections and Commissions which had not been published in the Comptes Rendus for economical reasons, are given hereafter, in compliance with the wishes expressed by officers of such Divisions, Sections and Commissions. Finally, some new information on IUPAC activities is given and a short report of the outcome of the Division Presidents' meeting is published.

22nd Bureau Meeting, October 29—30

The Executive Committee had decided that the 22nd Bureau Meeting will be convened, and the Division Presidents have proposed that their meeting be held on one day immediately after the Bureau Meeting. Consequently the entire Bureau will start its deliberations on Tuesday 29 October at 9 a.m. and will continue on Wednesday 30 October. The Division Presidents will have their meeting in addition on Thursday 31 October. This time schedule is now fixed and leaves possibilities for the Executive Committee Meeting on Monday 28 October, as well as on 1 November.

IUPAC 1918–1968

Ultimately everybody is informed hereby that 1968 is a jubilee year for the International Union of Pure and Applied Chemistry. The then President of the British Society of Chemical Industries, Sir WILLIAM POPE, visited in the summer 1918 his counterpart in Paris, Dr. P. Kestner the President of the Société des Industries chimiques de France, for a thorough discussion and cooperation. As a result of this first interview the International Union of Pure and Applied Chemistry was created in the autumn 1918 in the famous restaurant Coq d'Or in Stratton Street, London W1.

**ADDRESS OF PRESIDENT KONDRATIEV
AT THE OPENING CEREMONY OF THE 4th CONGRESS
OF CATALYSIS IN MOSCOW, JUNE 1968**

Ladies and Gentlemen!

I have the honour and pleasure of greeting, in the name of IUPAC, all participants of the Fourth International Congress on Catalysis and to wish you great success and fruitful work.

Catalysis, catalytic reactions represent the most essential and probably the greatest part of all chemical reactions. For this reason catalysis is of extreme importance for chemistry as a whole, and IUPAC, as an international body entrusted with coordination and treatment of all problems for which international agreement is necessary, certainly cannot stand apart from the problems of catalysis. IUPAC's interest to these problems manifests itself in including certain fields of catalysis in the programmes of IUPAC congresses. For instance, one of the sessions of the Moscow Congress in 1965 dealt with radiation catalysis. A number of Symposia sponsored by IUPAC were devoted to certain fields of catalysis or to related topics.

Moreover, the IUPAC Commission on Colloid and Surface Chemistry is concerned with certain problems of direct relation to catalysis, for example the terminology and symbols in the field of surface phenomena. However, all that is being done by IUPAC in this respect obviously is insufficient. In fact, despite the numerous discussions, the catalyticists did not yet reach agreement even on purely terminological questions, such as definition of the catalytic activity, the rate of a catalytic reaction, the rate constant, etc. Certainly this is the fault, first of all, of IUPAC that involves no body directly concerned with catalysis problems. Yet the fault of the catalyticists as such, first of all of the body called the International Congress on Catalysis, does not seem to be excluded. Besides organizing congresses it should raise problems for solution by IUPAC that was created with this aim.

I would like to express here the hope that all the abovementioned drawbacks in the relations between the International Congress on Catalysis and the IUPAC will soon be eliminated.

Let me wish once more great success to the Congress.

Thank you.

DETAILED INFORMATION REGARDING FORTHCOMING EVENTS

INTERNATIONAL SYMPOSIUM ON NATURAL PRODUCTS SYMPOSIUM INTERNACIONAL DE PRODUCTOS NATURALES

The International Union of Pure and Applied Chemistry (IUPAC) and the Mexican Chemical Society (SQM), are pleased to invite you to the International Symposium on Natural Products which will be held in Mexico City, Mexico from 21 to 25 April, 1969.

This Symposium will deal especially with steroids and terpenes and will take place according to the rules and program described below.

Submission of Papers

Original contributions related to the topics of the Symposium are invited. The presentations should be 15 to 20 minutes long, and a selection of the papers submitted will be made by the referees. Closing date for submission of papers is 1 November, 1968. An abstract of no more than 1000 words must accompany the paper submitted.

Plenary Lectures

The titles and authors of the Symposium lectures are as follows:

- L. TOLDY, Research Institute for Pharmaceutical Chemistry, Budapest (Hungary): The sidechain stereochemistry of some steroidal alkaloids
- R. DE GHENGI, Ayerst Laboratories, Montreal (Canada): Synthetic cardenolides and related products
- K. SCHREIBER, Institute for Plant Biochemistry, Berlin (Germany): Recent advances in the chemistry of plant steroids
- O. JEGGER, Eidg. Technische Hochschule, Zurich (Switzerland): Some novel transformations of steroids
- D. H. R. BARTON, Imperial College of Science and Technology, London (UK): Recent advances in steroid chemistry
- C. DJERASSI, Stanford University, California (USA): Applications of mass spectrometry in the steroid field
- K. TAKEDA, Shionogi Research Laboratories, Osaka (Japan): Sesquiterpenes containing an ether-linkage in the molecule
- J. ROMO, Instituto de Química, Universidad nacional autónoma de México (México, DF): Estudios recientes sobre sesquiterpenos

Information

All correspondence should be directed to "IUPAC-SQM Symposium" Sociedad química de México, Apartado postal 4-875. México 4 (DF México)

Official Languages

The official languages will be Spanish and English. There will be no simultaneous translation, but interpreters will be available to translate discussions from Spanish to English.

Publication

Abstracts of papers to be presented at the Symposium will be distributed in advance to all registrants.

XXVTH INTERNATIONAL CONFERENCE ON PURE AND APPLIED CHEMISTRY

Cortina d'Ampezzo 1st Decade of July 1969

IVTH INTERNATIONAL CONFERENCE ON ORGANOMETALLIC CHEMISTRY

Bristol, 27 July—1 August 1969

The Fourth International Conference on Organometallic Chemistry will be held in Bristol (UK), from 27 July to 1 August 1969, under the sponsorship of the Chemical Society of London, and the International Union of Pure and Applied Chemistry.

The Conference will be held at the School of Chemistry of the University of Bristol, and accommodation will be available in University Residence Halls. Accommodation for families will be available by private arrangement with local hotels.

A number of symposia will be held within the framework of the conference to allow more detailed discussion of certain topics. Suggestions for symposia topics will be welcome and may be given on the Preliminary Registration Form.

The number of papers to be presented at the Conference will probably have to be limited, and after Abstracts (due 1 March 1969, submitted in English) have been considered, invitations to present papers at the Conference will be issued. Authors may present papers in any language, but since simultaneous translation will not be available it would be preferred if English were used.

Address replies to the Secretary: Dr E.W. ABEL, School of Chemistry, University of Bristol, Cantock's Close, Bristol 8 (UK).

XXIIND INTERNATIONAL CONGRESS OF PURE AND APPLIED CHEMISTRY and XIITH INTERNATIONAL CONFERENCE ON COORDINATION CHEMISTRY

Sydney, 20–27 August, 1969

The Australian Academy of Science extends an invitation to a combined meeting, comprising the XXIInd International Congress of Pure and Applied Chemistry, and concurrently the XIIth International Conference on Coordination Chemistry, which will be held in Sydney, Australia, 20–27 August, 1969.

Scientific Programme XXIInd IUPAC Congress

The scientific programme will represent the interests of three Divisions of the International Union of Pure and Applied Chemistry—Physical Chemistry, Inorganic Chemistry, and Macromolecular Sciences, and will be presented under the following headings:

Physical Chemistry

1. Theoretical chemistry, and atomic and molecular spectroscopy (incorporating the Seventh Australian Spectroscopy Conference)
2. Intermolecular forces: solids, liquids, gases and solutions, *including a session on*
 - (a) Electrolytes and ionic melts
3. High pressure chemistry
4. Kinetics, *comprising*
 - (a) Reactions of free radicals and excited species
 - (b) Thermally-induced gas-phase reactions
 - (c) Kinetics at the solid/gas interface
 - (d) Rates and equilibria in solutions
5. The solid/liquid interface, *including sessions on*
 - (a) Electrode processes and the double layer
 - (b) Oxide-solution interfaces
6. *Symposium: 50 Years of Valence Theory (invited speakers only)*

Macromolecular Chemistry

1. Polymerization kinetics and the physical properties of polymers, *including sessions on*
 - (a) Graft polymerization
 - (b) Polyelectrolytes

Inorganic Chemistry

1. General inorganic chemistry, *comprising*
 - (a) Non-metals
 - (b) Non-transition metals
2. Mineral chemistry, *comprising*
 - (a) Interfacial processes in mineral extraction
 - (b) On-stream analysis in the mineral industry
3. Solid-state chemistry; *comprising*
 - (a) Preparation and growth of crystals, including vapour transport and hydrothermal synthesis
 - (b) Characterization, including defect solids and non-stoichiometric phases

XIIth International Conference on Coordination Chemistry

Papers will be presented under the following headings:

1. The nature of the metal-ligand bond in coordination complexes
2. Biological aspects of coordination chemistry
3. Mechanisms of substitution and electron-transfer reactions
4. Investigation of molecular dissymmetry
5. Complex equilibria in solution
6. Reactivity of coordinated ligands and catalysis by coordination compounds

7. Structure and reactivity of organometallic compounds

All scientific proceedings will take place in a compactly-sited group of lecture theatres in the University of Sydney. While the IUPAC and ICCC meetings will run concurrently, participants will be able to move freely from one to the other if they so wish.

In either programme the committee may accept papers of exceptional interest on topics other than those listed.

Plenary Lectures

The following have already accepted invitations to deliver plenary lectures: C.A.COULSON (UK), R.DAUDEL (France), B.V.DERJAGUIN (USSR), E.O.FISCHER (Germany), O.FOSS (Norway), E.U.FRANCK (Germany), D.H.FÜRSTENAU (USA), P.HAGENMULLER (France), J.O.HIRSCHFELDER (USA), J.JORTNER (Israel), B.B.MALMSTRÖM (Sweden), S.F.MASON (UK), R.S.MULLIKEN (USA), I.E.NEWMHAM (Australia), S.OKAMURA (Japan), C.SCHÄFFER (Denmark), H.TAUBE (USA), and G.WILKINSON (UK).

At least thirty invited Section Lectures will also be given.

Scientific Contributions

Those wishing to contribute papers are requested to indicate this on the preliminary application form. A title and abstract will be required when the final application form is returned; further details will appear in the second circular.

Registration

If you wish to attend you should complete the preliminary application form and mail it without delay. This will not commit you to attending, but return of the completed form will ensure that you receive further information and will greatly help the organizers. The second circular will be distributed later in 1968 to all those who have returned the preliminary application form. The registration fee will be \$27 (Australian currency) or US\$30 for active participants, and \$10 (Aust.) or US\$11 for students and accompanying members.

Correspondence

All correspondence concerning the meeting should be addressed to:
The Chairman, Organizing Committee, XXII IUPAC/XII ICCC
Box 2249U, G.P.O., Melbourne (Australia 3001)
Telex: 30236, Cables and Telegrams: Coresearch, Melbourne

Associated Meeting

An International Symposium on Electron and Nuclear Magnetic Resonance will be held at Monash University, Clayton, Victoria, under the auspices of the Australian Academy of Science, 11-14 August, 1969.

Further information concerning this Symposium can be obtained from The Executive Secretary, Australian Academy of Science, Gordon Street, Canberra City, A.C.T. (Australia 2601).

INTERNATIONAL SYMPOSIUM ON CONFORMATIONAL ANALYSIS

Brussels, 9-12 September 1969

List of lecturers of plenary lectures:

Prof. J. DALE, Oslo (Norway)
Prof. J. DUNITZ, Zürich (Switzerland)
Prof. E. L. ELIEL, Notre-Dame (USA)
Prof. R. U. LEMIEUX, Edmonton, Alberta (Canada)
Prof. K. MISLOW, Princeton (USA)
Prof. L. J. OOSTERHOFF, Leiden (Netherlands)
Dr J. OTH, Union Carbide, Brussels (Belgium)
Prof. A. RASSAT, Grenoble (France)
Prof. M. J. T. ROBINSON, Oxford (UK)
Prof. J. SICHER, Prague (Czechoslovakia)

SYMPOSIUM ON THE CHEMISTRY OF NATURAL PRODUCTS

Riga, June 1970

The Symposium sponsored by the IUPAC will be held in Riga in the last decade of June 1970. The organization of the Symposium has been undertaken by the USSR Academy of Sciences which has appointed for this purpose an Executive Committee (Chairman: Prof. YU. A. OVCHINNIKOV) and Scientific Programme Committee (Chairman: Prof. A. S. KHOKHLOV). The Honorary President of the Symposium will be Prof. M. M. SHEMYAKIN.

The Symposium will be devoted mainly to the chemistry of biologically active biopolymers and bio-regulators. Within the programme of the Symposium it is planned to hold 12 plenary lectures, including one dealing with a survey of recent Soviet work and to organize separate sections on the following topics:

- A. Chemistry of peptides and proteins
- B. Chemistry of nucleic acids and nucleotides
- C. Chemistry of lipids including the physical chemistry of membranes
- D. Chemistry of carbohydrates
- E. Chemistry of other natural products (steroids, antibiotics, alkaloids, terpenes, etc.)
- F. Physical methods

It is hoped that the following eminent scientists to whom invitations have been sent will give plenary lectures:

Prof. D. H. R. BARTON (UK), Prof. C. DJERASSI (USA), Prof. H. B. KHORANA (USA), Prof. D. E. KOSHLAND (USA), Prof. E. LEDERER (France), Prof. K. NAKANISHI (Japan), Prof. V. PRELOG (Switzerland), Prof. M. M. SHEMYAKIN (USSR), Prof. F. ŠORM (Czechoslovakia), Prof. F. B. STRAUB (Hungary), Prof. L. L. M. VAN DEENEN (Netherlands), and Prof. R. B. WOODWARD (USA).

It is also proposed to hold 3 Presymposium meetings especially devoted to the chemical aspects of (1) enzyme action, (2) biological membranes and (3) antibiotics.

The first circular containing information on the organizational matters of the Symposium will be issued this autumn.

All inquiries concerning the Symposium should be addressed to the General Secretary of Organizing Committee of the Symposium whose headquarters are in the Institute for Chemistry of Natural Products, Ul. Vavilova 32, Moscow, USSR.

I. DIVISION DE CHIMIE PHYSIQUE

Réunions du Comité de Division

1^{re} Réunion du mercredi 30 août 1967, 14 heures

Présents: Sir HARRY MELVILLE (président), Dr G. WADDINGTON (vice-président), Prof. T. FÖRSTER, Prof. J. TH. G. OVERBEEK, Prof. M. PRETTRE, Dr. H. A. SKINNER, Dr L. A. K. STAVELEY, Prof. G. EMSCHWILLER (secrétaire).

Excusé: Prof. A. N. FRUMKIN.

Invités à titre consultatif: Prof. M. L. MCGLASHAN, Prof. J. JORDAN, Prof. G. MILAZZO, Prof. R. C. LORD.

1 *Rapports des Commissions*

Des rapports verbaux sont présentés sur l'activité des différentes commissions. Les activités depuis la Conférence de Paris ont déjà été précédemment résumées (voir Information Bulletin 29, page 23).

Le Dr G. WADDINGTON, Président de la Commission I.1 des Symboles, Terminologie et Unités, expose les travaux de cette Commission qui s'est réunie les 28 et 29 août; ils sont résumés dans le rapport annexé plus loin. Il signale, en particulier, qu'une définition de la mole a été approuvée qui devra être transmise à la Commission internationale des Poids et Mesures.

Le Dr H. A. SKINNER, Président de la Commission I.2 de Thermodynamique et de Thermochimie traite spécialement de la question des publications de cette Commission et sollicite le concours financier de l'IUPAC pour le « Bulletin de Thermodynamique et de Thermochimie ». Il signale que la Commission prépare une liste de substances à tester pour la « rotating bomb calorimetry ».

L'activité de la Commission I.3 d'Electrochimie est présentée par le Prof. G. MILAZZO, délégué par cette Commission; il montre comment cette activité s'est développée tout à la fois dans trois domaines, celui de la cinétique électrochimique, celui de la thermodynamique électrochimique et celui de la nomenclature. Des questions relatives à l'enseignement de l'électrochimie ont également été abordées.

Sir HARRY MELVILLE, Président, signale qu'il a été décidé par le Conseil que la Commission I.4 de Chimie macromoléculaire serait réunie avec la Commission des Plastiques et des Hauts Polymères de la Division de Chimie Appliquée en une division nouvelle de Chimie macromoléculaire.

Le Dr L. A. K. STAVELEY, Président de la Commission I.5 des Données et Etalons physico-chimiques, expose l'activité de cette Commission et le début de ses travaux au cours de la matinée. Il traite en particulier les questions relatives à la caractérisation de pureté chimique. Une réunion de la Commission est envisagé pour 1968 et une somme de 600 US \$ demandée à cet effet.

Le Prof. R. C. LORD, Président de la Commission I.6 de Structure moléculaire et de Spectroscopie, expose l'activité de cette Commission et pose la question de la création de sections groupant plusieurs commissions, des contacts devront être pris avec la future Division de Chimie macromoléculaire.

Le Prof. J. TH. G. OVERBEEK, vice-président de la Commission I.7 de Chimie des Colloïdes et des Surfaces, présente le rapport d'activité de cette Commission qui ne compte plus maintenant que 2 Sous-Commissions et expose les projets d'activité à venir.

2 *Sort de la Commission de Chimie macromoléculaire*

Cette Commission disparaît du fait de la création de la Division de Chimie macromoléculaire.

3 *Maintien de la Commission d'Electrochimie*

Sir HARRY MELVILLE expose qu'une situation délicate a été créée du fait des positions non concordantes adoptées par le Bureau lors de sa réunion à Francfort les 24 et 25 février 1966 et par le Comité Exécutif lors de sa réunion à Scheveningen les 31 mars et 1^{er} avril 1967.

La Commission d'Electrochimie, lors de sa réunion du matin, a délégué les Proff. MILAZZO et JORDAN pour exposer les raisons qui militent en faveur de son maintien. Le Prof. MILAZZO précise, en particulier, combien les buts du CITCE et de l'IUPAC sont différents et qu'une des tâches de la Commission d'Electrochimie est de collecter les données de différente origine, qu'elles proviennent des travaux du CITCE ou des publications d'autres organismes.

Une discussion s'engage, à la suite de laquelle il est décidé à l'unanimité des membres présents du Comité de Division de proposer le maintien de la Commission d'Electrochimie dans l'intérêt même de l'IUPAC à laquelle doit appartenir toute décision finale en ce qui concerne la question de nomenclature, symboles, définitions, etc.

4 *Sort de la Commission de Structure moléculaire et de Spectroscopie*

Sir HARRY MELVILLE et le Prof. LORD exposent que cette Commission ne saurait faire double emploi avec la Commission Triple de Spectroscopie dont les buts et les tâches sont nettement différents et qu'en conséquence son maintien s'impose. Ce point de vue est adopté sans discussions.

5 *Commission de Haute Température et de Chimie de Plasmas*

A la réunion de Paris, il avait été suggéré que la Commission de Haute Température appartenant à la Division de Chimie inorganique soit rattachée à la Division de Chimie physique. Cette proposition n'avait pas été retenue par le Conseil. Puisque les problèmes d'échelles de température intéressent la Commission de Thermochimie, la question de la création d'une sous-commission a été posée à cette Commission. Le Dr SKINNER expose que les membres de cette Commission ont été unanimes à estimer, au cours d'une réunion tenue ce matin, que la création d'un groupe de travail chargé des problèmes appartenant à ce domaine apparaissait opportune. Le Comité de Division décide en conséquence la création de ce groupe au sein de la Commission I.2.

6 *Création d'un «Journal de Thermodynamique et de Thermochimie»*

Sir HARRY MELVILLE fait connaître que l'IUPAC ne peut accepter de subventionner des périodiques traitant de sujets d'intérêt particulier. Il est suggéré que la Commission soit représentée au Comité de rédaction et décide que le Dr SKINNER soumette des propositions à ce sujet.

II^e Réunion du jeudi 31 août 1967, 17 heures

Présents: Sir HARRY MELVILLE (président), Dr G. WADDINGTON (vice-président), Prof. T. FÖRSTER, Prof. J. TH. G. OVERBEEK, Prof. M. PRETTRE, Dr H. A. SKINNER, Dr L. A. K. STAVELEY, Prof. G. EMSCHWILLER (secrétaire).

Excusé: Prof. A. N. FRUMKIN.

Invités: Prof. M. L. MCGLASHAN, Prof. P. VAN RYSSELBERGHE.

7 *Elections*

Le Comité de Division ratifie les propositions pour la nouvelle composition des commissions, à la suite des élections, auxquelles elles ont procédé. Le Dr D. R. STULL est nommé membre du Comité de Division en remplacement du Dr L. A. K. STAVELEY dont le mandat est arrivé cette année à expiration.

8 Propositions des Commissions

Le Dr SKINNER, revenant sur la création d'un groupe de travail sur la chimie de plasmas, précise qu'un colloque est prévu qui réunira 15 à 20 spécialistes dans ce domaine avant 1969. Sir HARRY MELVILLE signale qu'il y aurait intérêt à reporter ce colloque à 1969 pour des raisons de disponibilités financières.

I.1 Commission on Symbols, Terminology and Units

The Commission met on 28 and 29 August 1967 in Prague from 9–12.30 and 14–18 h each day. The Commission had also met on 20, 21, 22 December 1963 in Paris.

Present at the Prague meetings were: Members: GUY WADDINGTON (Chairman), M. L. MCGLASHAN (Vice-Chairman), H. BRUSSET (Secretary), R. BATES, W. JAENICKE, K. J. PEDERSEN, E. H. WIEBENGA.

Absent: M. MILONE and K. V. ASTACHOV.

Present as Observers: M. A. PAUL (USA), M. ROUDNÝ (Czechoslovakia).

The semi-final draft Manual of Symbols and Terminology for Physicochemical Quantities and Units was reviewed completely. Comments from other Commissions and individuals, as well as from Commission members were considered and when appropriate were adopted. A new draft incorporating all improvements will be prepared and recirculated to Commission Members (STU) by 15 October 1967 for rapid review. Final comments will then be incorporated in the Tentative Manual to be published in the Information Bulletin, hopefully by about December 1967, for distribution to all IUPAC people including adhering organizations. After 8 months all additional comments received will be incorporated in the Manual if they are suitable.

A document entitled Activity Coefficients will be included in the Manual as an Appendix. If it is well received it will be published in the final version.

If comments on the Bulletin version are numerous, a special meeting of the Commission may be necessary. Costs of such a meeting are estimated at about 2000 \$ and the Division is asked to budget this amount.

Two points about the final publication are noted: (1) A French version will be included; (2) wide distribution should be brought about by translation into languages other than French and English and by reprinting without restrictions in various scientific journals.

In the Manual there appears the following definition of the mole:

"Mole: The mole is an amount of substance of a system which contains as many elementary units as there are carbon atoms in 0.012 kg (exactly) of the pure nuclide ^{12}C . The elementary unit must be specified and may be an atom, a molecule, an ion, an electron, a photon, etc., or a specified group of such entities."

The same definition has been accepted by the SUN Commission of IUPAC and by ISO. It is currently being seriously considered by the Comité International de Poids et Mesures (CIPM) for adoption as a seventh basic unit of the Système International. IUPAC is asked to endorse the above definition and to inform COPM of this endorsement (an earlier version of the definition was approved by the Bureau of IUPAC (date).)

The Commission documents on symbols and nomenclature for the fields of (1) spectrochemical analysis and (2) colloid and surface chemistry prepared by the respective Commissions (V.4 and I). Both documents are important and should be published after additional review. Commission I.1 points out its important role in reviewing symbols documents from other IUPAC Com-

missions which it has because of its central position and close links with other international bodies.

The Commission in looking at its future sees many important tasks such as (1) a new manual with more attention to definitions and systematization of the use of units, (2) symbols for quantum chemistry, (3) symbols for chemical engineering, (4) essay type documents needed to clarify in a number of areas, e.g. standard states and equilibrium constants.

Membership: Terms of office of 5 members expired. They are: BRUSSET, PEDERSEN, MILONE, WIEBENGA and WADDINGTON. Surviving members are: BATES, ASTACHOV, JAENICKE, MCGLASHAN. Three new members have been elected subject to confirmation: They are: FAYART (France), MASIA (Spain), M. A. PAUL (USA), SILLÉN (Sweden), and JELLINEK (Netherlands). G. WADDINGTON was elected an Associate Member. M. L. MCGLASHAN and M. A. PAUL were elected Chairman and Secretary respectively.

I.3 Commission on Electrochemistry

Synopsis of objectives, policies and proposed activities for the biennium 1967-69

1 Objectives

Topics of international scientific and technical significance will be studied, with the aim to facilitate advances in the field of electrochemistry. In the wake of recent theoretical developments, a critical tabulation and interpretation of thermodynamic and kinetic data (available in the literature) will be undertaken. Retrieval and re-interpretation of a wealth of information is thus envisioned. A comprehensive compendium of data will be compiled and made available to the international community of several thousand scientists active in fundamental research in electrochemistry and important applications (e.g. fuel cells). Guidelines will be developed for the design of mechanistically significant experiments on electrode processes, in the light of contemporary knowledge of diffusion theory, physicochemical hydrodynamics, electric double layer theory, etc.

Matters of nomenclature and symbols in the areas of electrochemical thermodynamics and kinetics will be given appropriate attention. Relevant proposals for the standardization and codification of terminology will be submitted for consideration by appropriate IUPAC bodies.

2 Policies

The Commission on Electrochemistry will have a membership broadly representative of the international community of scientists engaged in significant activities in the field of electrochemistry. The Commission will maintain channels of direct communication and cooperation with interested individuals and associations (e.g. electrochemical societies in various countries, the Faraday Society, Comité International de Thermodynamique et Cinétique Electrochimiques (CITCE)). However, *all matters concerning symbols and terminology will be referred by the Commission on Electrochemistry to the Commission on Physico-Chemical Symbols and Terminology, prior to dissemination*. It is understood that dissemination of norms affecting terminology and symbols will be subject to IUPAC approval recommended by the Commission on Physico-Chemical Symbols and Terminology. Consultation with that Commission as well as with the Commission on Electroanalytical Chemistry will be maintained via groups of three members of the Commission on Electrochemistry, delegated ad-hoc.

I.5 Commission on Molecular Structure and Spectroscopy

The Effect on Chemical Spectroscopy of the Adoption of the International System of Units (SI System)

The Commission on Molecular Structure and Spectroscopy at Technical Sessions, held at Madrid on 9/10 September 1967 considered the implications to chemical spectroscopy of the adoption of the SI System of Units. The Commission recognized the desirability of establishing a self-consistent system of units and symbols for the physical sciences, and that to be effective such a system must be fully supported by the International Unions. At the same time, it noted with concern that the introduction of the SI System would create difficulties for spectroscopists because the adoption into general use of some of the units would run contrary to long established and universal practice: in some cases the self-consistency would seemingly constitute the sole merit of the new unit over that currently in universal use. Singled out for particular comment in this context is the recommended phasing out of the Ångström unit in favor of the nanometre as a measure of molecular bond distances and wavelength, and the replacement of the reciprocal centimetre (cm^{-1}) by the reciprocal metre (m^{-1}) as a unit of wavenumber.

It was the unanimous opinion of the Commission that a doctrinaire attempt to induce spectroscopists to accept the SI Unit System *in toto* (as for example by the Editorial Boards of chemical journals) would create irritation and tend to polarize feelings against the meritorious features of the SI System. This would be unfortunate, since the acceptance or rejection of the SI System should be based on its merit, unimpeded by prejudice, *pro* or *con*.

The view was strongly expressed that decisions affecting the units and terminology of spectroscopy should be referred to the ICSU Joint Commission for Spectroscopy before any action is taken.

Ottawa, 17 January 1968

R. N. JONES, Chairman
Commission on Molecular
Structure and Spectroscopy

PHYSICAL CHEMISTRY DIVISION

Commission on Symbols, Terminology, and Units

DRAFT OF AN EXTENSIVELY REVISED VERSION OF THE 1959 "MANUAL OF PHYSICOCHEMICAL SYMBOLS AND TERMINOLOGY"

Note: Comments on this draft should be sent within eight months of its publication in this journal to the Chairman of the Commission: Professor M.L. McGlashan, Department of Chemistry, The University of Exeter, Stocker Road, Exeter, Devon, UK. The draft will then be reviewed once more by the Commission in the light of comments received, and will then be submitted to the Division for its approval before final publication.

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Preface

The Commission on Symbols, Terminology, and Units is a part of the Division of Physical Chemistry of the International Union of Pure and Applied Chemistry. Its general responsibilities are to secure clarity and precision, and wider agreement in the use of symbols, by chemists in different countries, and among physicists, chemists, and engineers, and by editors of scientific

journals. In pursuing these aims, liaison is maintained with other international organizations and in particular with the Commission on Symbols, Units and Nomenclature of the International Union of Pure and Applied Physics (SUN Commission) and Technical Committee 12 of the International Organization for Standardization (ISO/TC 12). References to the publications of these two organizations are given in 12.1 and 12.2 of this Manual. These publications may be referred to for more extended coverage of symbols for quantities, and related information, not commonly used by chemists. The recommendations presented here are generally in agreement with those of the SUN Commission and ISO/TC 12.

The present publication supersedes the Commission's publication of 1959 (Reference 12.3) in English and French and its translations into other languages.

1. Physical Quantities and Symbols for Physical Quantities

1.1 *Physical quantities*

A *physical quantity* is the product of a *numerical value* (a pure number) and a *unit*. For many dimensionless physical quantities the unit has no name or symbol and is not explicitly indicated.

1.2 *Printing of symbols for physical quantities*

The symbols for physical quantities should be single letters[◊] of the Latin or Greek alphabets which, when necessary, may be modified by subscripts and/or superscripts of specified meaning. The symbols for physical quantities should always be printed in italic (sloping) type.

The symbols for vector quantities should be printed in bold-faced italic type.

1.3 *Printing of subscripts and superscripts*

Subscripts or superscripts which are themselves symbols for physical quantities should be printed in italic (sloping) type and all others in roman (upright) type.

Example: C_p for heat capacity at constant pressure, but
 C_B for heat capacity of substance B

1.4 *Products and quotients of physical quantities*

A product of two quantities a and b may be represented in any of the ways:

$$ab \text{ or } a \cdot b \text{ or } a . b \text{ or } a \times b$$

and their quotient in any of the ways:

$$\frac{a}{b} \text{ or } a/b \text{ or } ab^{-1}$$

or in any of the other ways of writing the product of a and b^{-1} .

Example: Reynolds number: (Re)

These rules may be extended to more complex groupings but more than one solidus (/) should never be used in the same expression unless parentheses are used to eliminate ambiguity.

Example: $(a/b)/c$ or $a/(b/c)$ but never $a/b/c$

[◊] An exception to this rule has been made for certain dimensionless quantities used in the study of transport processes (see Section 2.9), for which the internationally agreed symbols consist of two letters. Such two-letter symbols should be enclosed in parentheses.

2. Recommended Names and Symbols for Quantities in Chemistry and Physics

Remarks: Where two or more symbols are indicated for a given quantity and are separated only by commas (without parentheses), they are on an equal footing; symbols within parentheses are secondary recommendations.

In the following list any description given after the name of a physical quantity is merely for identification and is not intended to be a complete definition.

Vector notation is used where appropriate in Section 2.6; it may be used when convenient also for appropriate quantities in other sections.

The word "specific" before the name of an extensive physical quantity is restricted to the meaning "divided by mass". For example specific volume is the volume divided by the mass. When the extensive quantity is represented by a capital letter, the corresponding specific quantity may be represented by the corresponding lower case letter.

<i>Examples:</i> volume: V	specific volume: $v = V/m$
heat capacity: C_p	specific heat capacity: $c_p = C_p/m$

The word "molar" before the name of an extensive quantity is restricted to the meaning "divided by amount of substance". For example molar volume is the volume divided by the amount of substance. The subscript m attached to the symbol for the extensive quantity denotes the corresponding molar quantity.

<i>Examples:</i> volume: V	molar volume: $V_m = V/n$
Gibbs energy: G	molar Gibbs energy: $G_m = G/n$

The subscript m may be omitted when there is no risk of ambiguity.

The symbol X_B , where X denotes an extensive quantity and B is the chemical symbol for a substance, denotes the partial molar quantity of the substance B defined by the relation:

$$X_B = (\partial X / \partial n_B)_{T, p, n_C, \dots}$$

For a pure substance B the partial molar quantity X_B and the molar quantity X_m are identical. The partial molar quantity X_B of pure substance B, which is identical with the molar quantity X_m of pure substance B, may be denoted by X_B^\bullet , where the superscript \bullet denotes "pure", so as to distinguish it from the partial molar quantity X_B of substance B in a mixture.

2.1 *Space, time, and related quantities*

2.1.01	length	l
2.1.02	height	h
2.1.03	radius	r
2.1.04	diameter	d
2.1.05	path, length of arc	s
2.1.06	wavelength	λ
2.1.07	wavenumber: $\sigma = 1/\lambda$	$\sigma, \bar{\nu}$
2.1.08	plane angle	$\alpha, \beta, \gamma, \theta, \phi$
2.1.09	solid angle	ω, Ω
2.1.10	area	A, S
2.1.11	volume	V

2.1.12	time	t
2.1.13	frequency	ν, f
2.1.14	angular frequency, pulsance: $2\pi\nu$	ω
2.1.15	period: $1/\nu$	T
2.1.16	characteristic time interval, relaxation time, time constant	τ
2.1.17	velocity	v, u, w, c
2.1.18	angular velocity: $d\phi/dt$	ω
2.1.19	acceleration	a
2.1.20	acceleration of free fall	g

2.2 *Mechanical and related quantities*

2.2.01	mass	m
2.2.02	reduced mass	μ
2.2.03	specific volume (volume divided by mass)	v
2.2.04	density (mass divided by volume)	ρ
2.2.05	relative density (ratio of the density to that of a reference substance)	d
2.2.06	moment of inertia	I
2.2.07	momentum	p
2.2.08	force	F
2.2.09	weight	$G, (W)$
2.2.10	moment of force	M
2.2.11	angular momentum	L
2.2.12	work (force times path)	w, W
2.2.13	energy	E
2.2.14	potential energy	E_p, V, Φ
2.2.15	kinetic energy	E_k, T, K
2.2.16	Hamiltonian function	H
2.2.17	Lagrangian function	L
2.2.18	power (energy divided by time)	P
2.2.19	pressure	p, P
2.2.20	normal stress	σ
2.2.21	shear stress	τ
2.2.22	linear strain (relative elongation): $\Delta l/l_0$	ε, e
2.2.23	volume strain (bulk strain): $\Delta V/V_0$	θ
2.2.24	modulus of elasticity (normal stress divided by linear strain, Young's modulus)	E
2.2.25	shear modulus (shear stress divided by shear angle)	G
2.2.26	compressibility: $-V^{-1}(dV/dp)$	κ
2.2.27	compression (bulk) modulus: $p = -K\Delta V/V_0$	K
2.2.28	velocity of sound	c
2.2.29	viscosity	$\eta, (\mu)$
2.2.30	fluidity: $1/\eta$	ϕ
2.2.31	kinematic viscosity: η/ρ	ν
2.2.32	friction coefficient (frictional force divided by normal force)	$\mu, (f)$
2.2.33	surface tension	γ, σ
2.2.34	angle of contact	θ
2.2.35	diffusion coefficient	D
2.2.36	mass transfer coefficient (mass divided by time and by cross-sectional area)	k, k_m

2.3	<i>Molecular and related quantities</i>	
2.3.01	relative atomic mass of an element (also called "atomic weight") [†]	A_r
2.3.02	relative molecular mass of a substance (also called "molecular weight") ^{††}	M_r
2.3.03	mass of one molecule	m
2.3.04	molar mass (mass divided by amount of substance)	M
2.3.05	Avogadro constant	L, N_A
2.3.06	number of molecules	N
2.3.07	amount of substance	$n, (v)$
2.3.08	mole fraction of substance B: $n_B/\sum_B n_B$	x_B, y_B
2.3.09	mass fraction of substance B	w_B
2.3.10	volume fraction of substance B	ϕ_B
2.3.11	molality of solute substance B (amount of B divided by mass of solvent) ^{†††}	m_B
2.3.12	concentration of solute substance B (amount of B divided by the volume of the solution) ^{††††}	$c_B, [B]$
2.3.13	surface concentration, surface excess	Γ
2.3.14	mass concentration of substance B (mass of B divided by the volume of the solution)	ρ_B
2.3.15	molecular concentration of substance B (number of molecules or particles divided by volume)	c_B, n_B

[†] The ratio of the average mass per atom of the natural isotopic composition of an element to 1/12 of the mass of an atom of nuclide ^{12}C .

Example: $A_r(\text{Cl}) = 35.453$

The concept of relative atomic mass may be extended to other specified isotopic compositions, but the natural isotopic composition is assumed unless some other composition is specified.

^{††} The ratio of the average mass per molecule of the natural isotopic composition of a substance to 1/12 of the mass of an atom of nuclide ^{12}C .

Example: $M_r(\text{KCl}) = 74.555$

The concept of relative molecular mass may be extended to other specified isotopic compositions, but the natural isotopic composition is assumed unless some other composition is specified.

^{†††} A solution having a molality equal to 0.1 mol kg⁻¹ say, is sometimes called a 0.1 molal solution or a 0.1 m solution. However "molal" is not recognized as a unit-symbol in the International System of Units (SI) (see Section 3) and its use is accordingly discouraged. The letter m is the SI unit-symbol for the metre; its use as an abbreviation for mol kg⁻¹ must therefore be strongly deprecated.

^{††††} Concentration is sometimes called "molarity" but this name is both unnecessary and liable to cause confusion with molality, and is therefore not recommended.

A solution with a concentration of 0.1 mol dm⁻³ say, is sometimes called a 0.1 molar solution or a 0.1 M solution. However, neither "molar" nor "M" is recognized as a unit-symbol in the International System of Units (SI) (see Section 3) and their use is accordingly discouraged. The use of "molar" as an abbreviation for mol dm⁻³ is particularly discouraged in view of the agreed use of this word in the names of physical quantities with the meaning "divided by amount of substance" (see p.6). The abbreviation "M" for mol dm⁻³ should never be used except for rough values in aqueous solutions because of possible confusion between mol dm⁻³ and mol kg⁻¹.

2.3.16	collision diameter of a molecule	d, σ
2.3.17	mean free path	l, λ
2.3.18	collision number (number of collisions divided by volume and by time)	Z
2.3.19	grand partition function (system)	Ξ
2.3.20	partition function (system)	Q, Z
2.3.21	partition function (particle)	q, z
2.3.22	statistical weight	g
2.3.23	symmetry number	σ, s
2.3.24	characteristic temperature	Θ
2.4	<i>Thermodynamic and related quantities</i>	
2.4.01	thermodynamic temperature, absolute temperature	$T, (\Theta)$
2.4.02	customary temperature (on the Celsius, Fahrenheit, or other practical scale)	t, θ
2.4.03	molar gas constant	R
2.4.04	Boltzmann constant	k
2.4.05	heat	q, Q
2.4.06	work	w, W
2.4.07	internal energy	$U, (E)$
2.4.08	enthalpy: $U + pV$	H
2.4.09	entropy	S
2.4.10	Helmholtz energy: $U - TS$	A
2.4.11	Massieu function: $(-A/T)$	J
2.4.12	Gibbs energy: $H - TS$	G
2.4.13	Planck function: $(-G/T)$	Y
2.4.14	compression factor: pV_m/RT	Z
2.4.15	heat capacity	C
2.4.16	specific heat capacity (heat capacity divided by mass; the name "specific heat" is not recommended)	c
2.4.17	ratio C_p/C_v	γ, κ
2.4.18	chemical potential of substance B	μ_B
2.4.19	absolute activity of substance B: $\exp(\mu_B/RT)$	λ_B
2.4.20	fugacity	f, p^*
2.4.21	osmotic pressure	Π
2.4.22	ionic strength: $I_m = \frac{1}{2} \sum_i m_i z_i^2$ or $I_c = \frac{1}{2} \sum_i c_i z_i^2$	I
2.4.23	activity, relative activity of substance B	a_B
2.4.24	activity coefficient, mole fraction basis	f_B
2.4.25	activity coefficient, molality basis	γ_B
2.4.26	activity coefficient, concentration basis	y_B
2.4.27	osmotic coefficient	g, ϕ
2.4.28	Joule-Thomson coefficient	μ
2.4.29	thermal conductivity	λ, k
2.4.30	thermal diffusivity: $\lambda/\rho c_p$	a
2.4.31	coefficient of heat transfer (density of heat flow rate divided by temperature difference)	h
2.4.32	cubic expansion coefficient: $V^{-1}(\partial V/\partial T)_p$	α
2.4.33	isothermal compressibility: $-V^{-1}(\partial V/\partial p)_T$	κ
2.4.34	pressure coefficient: $(\partial p/\partial T)_V$	β
2.5	<i>Chemical reactions</i>	
2.5.01	stoichiometric coefficient of substance B (negative for reactants, positive for products)	ν_B
2.5.02	general equation for a chemical reaction	$0 = \sum_B \nu_B B$
2.5.03	extent of reaction: $d\xi = dn_B/\nu_B$	ξ

2.5.04	rate of reaction: $d\xi/dt$ (see page 39)	$\dot{\xi}, J$
2.5.05	rate of increase of concentration of substance B: dc_B/dt	v_B, r_B
2.5.06	rate constant	k
2.5.07	affinity of a reaction: $(-\sum_B v_B \mu_B)$	$A, (\mathcal{A})$
2.5.08	equilibrium constant	K
2.5.09	reaction product (of the same form as K , but for non-equilibrium conditions)	Q
2.5.10	degree of dissociation	α
2.6	<i>Electricity and magnetism</i>	
2.6.01	elementary charge	e
2.6.02	quantity of electricity	Q
2.6.03	charge density	ϱ
2.6.04	surface charge density	σ
2.6.05	electric current	I
2.6.06	electric current density	j
2.6.07	electric potential	V, ϕ
2.6.08	electric tension: $U = IR$	U
2.6.09	electric field strength	E
2.6.10	electric displacement	D
2.6.11	capacitance	C
2.6.12	permittivity: $D = \epsilon E$	ϵ
2.6.13	permittivity of vacuum	ϵ_0
2.6.14	relative permittivity: ϵ/ϵ_0	$\epsilon_r, (\epsilon)$
2.6.15	dielectric polarization: $D - \epsilon_0 E$	P
2.6.16	electric susceptibility: $\epsilon_r - 1$	χ_e
2.6.17	electric dipole moment	p, p_e
2.6.18	permanent dipole moment of a molecule	p
2.6.19	induced dipole moment of a molecule	p, p_i
2.6.20	electric polarizability of a molecule	α
2.6.21	magnetic field strength	H
2.6.22	magnetic flux density, magnetic induction	B
2.6.23	permeability: $B = \mu H$	μ
2.6.24	permeability of vacuum	μ_0
2.6.25	relative permeability: μ/μ_0	μ_r
2.6.26	magnetization: $B/\mu_0 - H$	M
2.6.27	magnetic susceptibility: $\mu_r - 1$	$\chi, (\chi_m), (K)$
2.6.28	Bohr magneton	μ_B
2.6.29	electromagnetic moment: $E_p = -m \cdot B$	m, μ
2.6.30	resistance	R
2.6.31	resistivity (formerly called specific resistance): $E = \varrho j$	ϱ
2.6.32	conductivity (formerly called specific conductance): $j = \kappa E$	$\kappa, (\sigma)$
2.6.33	self-inductance	L
2.6.34	mutual inductance	M, L_{12}
2.6.35	reactance	X
2.6.36	impedance (complex impedance): $R + iX$	Z
2.6.37	loss angle	δ
2.6.38	admittance (complex admittance): $1/Z = G + iB$	Y
2.6.39	conductance	G
2.6.40	susceptance	B

† Also called dielectric constant and denoted by D when it is independent of E .

2.7	<i>Electrochemistry</i>	
2.7.01	Faraday constant	F
2.7.02	charge number of an ion B (positive for cations, negative for anions)	z_B
2.7.03	charge number of a cell reaction	z
2.7.04	electromotive force	E
2.7.05	electrochemical potential of ionic component B: $(\mu_B + z_B F \phi)$	$\tilde{\mu}_B$
2.7.06	electric mobility (velocity divided by electric field strength)	u, μ
2.7.07	electrolytic conductivity (formerly called specific conductance)	$\kappa, (\sigma)$
2.7.08	molar conductivity of electrolyte or ion: κ/c	Λ, λ
2.7.09	transport number (transference number or migration number)	t
2.7.10	overpotential, overtension (also called "overvoltage")	η
2.7.11	exchange current density	j_0
2.7.12	electrochemical transfer coefficient	α
2.7.13	strength of double layer (moment divided by area)	τ
2.7.14	electrokinetic potential (zeta potential): τ/ϵ	ζ
2.7.15	thickness of diffusion layer	δ
2.7.16	inner electric potential	ϕ
2.7.17	outer electric potential	ψ
2.7.18	surface electric potential difference: $\phi - \psi$	χ
2.8	<i>Light and related electromagnetic radiation</i>	
2.8.01	Planck constant	h
2.8.02	Planck constant divided by 2π	\hbar
2.8.03	radiant energy	$Q \quad \diamond$
2.8.04	radiant flux, radiant power	$\Phi \quad \diamond$
2.8.05	radiant intensity: $d\Phi/d\omega$	$I \quad \diamond$
2.8.06	radiance: $dI/dS \cos \theta$	$L \quad \diamond$
2.8.07	radiant emittance: $d\Phi/dS$	$M \quad \diamond$
2.8.08	irradiance: $d\Phi/dS$	$E \quad \diamond$
2.8.09	absorption factor (ratio of absorbed to incident radiant or luminous flux)	α
2.8.10	reflection factor (ratio of reflected to incident radiant or luminous flux)	ρ
2.8.11	transmission factor (ratio of transmitted to incident radiant or luminous flux)	τ
2.8.12	transmittance: $T = I/I_0$	T
2.8.13	Napierian absorbance (Napierian extinction): $B = \ln(1/T)$	B
2.8.14	Napierian absorptivity (Napierian absorption or extinction coefficient): $b = B/l$	b

◊ The word molar, contrary to the general rule given on p.6, here means "divided by concentration".

◊ The same symbol is often used also for the corresponding luminous quantity. Subscripts e for energetic and v for visible may be added whenever confusion between these quantities might otherwise occur.

2.8.15	molar Napierian absorptivity (molar Napierian absorption or extinction coefficient): $\kappa = B/lc$	κ
2.8.16	decadic absorbance (decadic extinction): $A = \log_{10}(1/T)$	A
2.8.17	decadic absorptivity (decadic absorption or extinction coefficient): $a = A/l$	a
2.8.18	molar decadic absorptivity (molar decadic absorption or extinction coefficient): $\epsilon = A/lc$	ϵ
2.8.19	quantum yield	Φ
2.8.20	exposure: $\int E dt$	H
2.8.21	speed of light in vacuo	c
2.8.22	refractive index	n
2.8.23	molar refraction: $(n^2 - 1) V_m/(n^2 + 2)$	R_m
2.8.24	angle of optical rotation	α

2.9 *Transport properties* $\diamond\diamond$

2.9.01	flux (of a quantity X)	J_X, J
2.9.02	Reynolds number: $\rho v l / \eta$	(Re)
2.9.03	Euler number: $p / \rho v^2$	(Eu)
2.9.04	Froude number: $v / (lg)^{\frac{1}{2}}$	(Fr)
2.9.05	Grashof number: $l^3 g \alpha \Delta \theta \rho^2 / \eta^2$	(Gr)
2.9.06	Weber number: $\rho v^2 l / \gamma$	(We)
2.9.07	Mach number: v / c	(Ma)
2.9.08	Knudsen number: λ / l	(Kn)
2.9.09	Strouhal number: lf / v	(Sr)
2.9.10	Fourier number: $a \Delta t / l^2$	(Fo)
2.9.11	Peclet number: vl / a	(Pe)
2.9.12	Rayleigh number: $l^3 g \alpha \Delta \theta \rho / \eta a$	(Ra)
2.9.13	Nusselt number: hl / k	(Nu)
2.9.14	Stanton number: $h / \rho v c_p$	(St)
2.9.15	Fourier number for mass transfer: Dt / l^2	(Fo^*)
2.9.16	Peclet number for mass transfer: vl / D	(Pe^*)
2.9.17	Grashof number for mass transfer: $- l^3 g (\partial \rho / \partial x)_{T, p} \Delta x \rho / \eta^2$	(Gr^*)
2.9.18	Nusselt number for mass transfer: $k_m l / \rho D$	(Nu^*)
2.9.19	Stanton number for mass transfer: $k_m / \rho v$	(St^*)
2.9.20	Prandtl number: $\eta / \rho a$	(Pr)
2.9.21	Schmidt number: $\eta / \rho D$	(Sc)
2.9.22	Lewis number: a / D	(Le)
2.9.23	Magnetic Reynolds number: $v \mu \kappa l$	(Re_m)
2.9.24	Alfvén number: $vl(\rho \mu)^{\frac{1}{2}} / B$	(Al)
2.9.25	Hartmann number: $B l (\kappa / \eta)^{\frac{1}{2}}$	(Ha)
2.9.26	Cowling number: $B^2 / \mu \rho v^2$	(Co)

\diamond The word molar, contrary to the general rule given on p.6, here means "divided by concentration".

$\diamond\diamond$ References to the symbols used in defining the dimensionless parameters 2.9.02 to 2.9.26 are as follows:

Q	2.2.04	v	2.1.17	l	2.1.01	η	2.2.29	p	2.2.19
g	2.1.20	α	2.4.32	θ	2.4.02	γ	2.2.33	c	2.2.28
λ	2.3.17	f	2.1.13	a	2.4.30	t	2.1.12	h	2.4.31
k	2.4.29	c_p	2.4.16	D	2.2.35	x	2.3.08	k_m	2.2.36
μ	2.6.23	κ	2.6.32	B	2.6.22				

It is much more difficult to make detailed recommendations on symbols for particular cases of physical quantities than on symbols for the general cases. The reason is the incompatibility between the need for specifying numerous details and the need for keeping the printing reasonably simple. Among the most awkward things to print are superscripts to subscripts and subscripts to subscripts. Examples of symbols to be avoided are:

$$\Lambda_{\text{NO}_3^-} \quad \Delta H_{25^\circ\text{C}} \quad (pV)_{0^\circ\text{C}}^{p=0}$$

The problem is vastly reduced if it is recognized that two different kinds of notation are required for two different purposes. In the formulation of general fundamental relations the most important requirement is a notation which is easy to understand and easy to remember. In applications to particular cases, in quoting numerical values, and in tabulation, the most important requirement is complete elimination of any possible ambiguity even at the cost of an elaborate notation.

The advantage of a dual notation is already to some extent accepted in the case of concentration. The recommended notation for the formulation of the equilibrium constant K_c for the general reaction:

$$0 = \sum_B \nu_B B$$

is

$$K_c = \prod_B (c_B)^{\nu_B}$$

but when we turn to a particular example it is better to use a notation such as:



$$\frac{[\text{HOBr}][\text{H}^+][\text{Br}^-]}{[\text{Br}_2]} = K_c$$

$$K_c(25^\circ\text{C}) = 6 \times 10^{-9} \text{ mol}^2 \cdot \text{dm}^{-6}$$

Once the principle of dual notation is accepted, its adaptability and usefulness become manifest in all fields of physical chemistry. It will here be illustrated by just a few examples.

The general relation between the molar conductivity of an electrolyte and the molar conductivities of the two ions is written most simply and most clearly as:

$$\Lambda = \Lambda^+ + \Lambda^-$$

but when it comes to giving values in particular cases a much more appropriate notation is:

$$\begin{aligned} \Lambda(\tfrac{1}{2}\text{Mg}^{2+}) &= 53 \Omega^{-1} \cdot \text{cm}^2 \cdot \text{mol}^{-1} \text{ at } 25^\circ\text{C} \\ \Lambda(\text{Cl}^-) &= 76 \Omega^{-1} \cdot \text{cm}^2 \cdot \text{mol}^{-1} \text{ at } 25^\circ\text{C} \\ \Lambda(\tfrac{1}{2}\text{MgCl}_2) &= 129 \Omega^{-1} \cdot \text{cm}^2 \cdot \text{mol}^{-1} \text{ at } 25^\circ\text{C} \\ \Lambda(\text{MgCl}_2) &= 258 \Omega^{-1} \cdot \text{cm}^2 \cdot \text{mol}^{-1} \text{ at } 25^\circ\text{C} \end{aligned}$$

The general relation between the partial molar volumes of the two components A and B of a binary mixture is written most simply:

$$n_A dV_A + n_B dV_B = 0 \quad (T, p \text{ const.})$$

But when it comes to specifying values, a completely different notation is called for, such as:

$$V(\text{K}_2\text{SO}_4, 0.1 \text{ mol} \cdot \text{dm}^{-3} \text{ in } \text{H}_2\text{O}, 25^\circ\text{C}) = 48 \text{ cm}^3 \cdot \text{mol}^{-1}$$

Each kind of notation is appropriate to its purpose.

A last example will be given relating to optical rotation. The relations between the angle α of rotation of the plane of polarization and the amount n , or the number N of molecules, of the optically active substance in the path of a light beam of cross-section A can be clearly expressed in the form:

$$\alpha = n\alpha_n/A = N\alpha_N/A$$

where α_n is the molar optical rotatory power and α_N the molecular optical rotatory power. When on the other hand it is desired to record an experimental measurement, an appropriate notation would be:

$$\alpha(5893 \text{ \AA}, 20^\circ\text{C, sucrose, } 10 \text{ g} \cdot \text{dm}^{-3} \text{ in } \text{H}_2\text{O, } 10 \text{ cm}) = + 66.470^\circ$$

2.11 *Recommended superscripts*

The following superscripts are recommended.

- pure substance
- $^\infty$ infinite dilution
- ^{1d} ideal
- $^\ominus$ standard in general \diamond
- † pressure independent term
- ‡ transition state, activated complex

3. **Units and Symbols for Units**

3.1 *Printing of symbols for units*

The symbol for a unit should be printed in roman (upright) type, should remain unaltered in the plural, and should not be followed by a full stop except when it occurs at the end of a sentence in text.

Example: 5 cm but not 5 cms and not 5 cm. and not 5 cms.

The symbol for a unit derived from a proper name should begin with a capital roman (upright) letter.

Examples: J for joule and Hz for hertz

Any other symbol for a unit should be printed in lower case Roman (upright) type.

3.2 *Printing of prefixes*

Symbols for prefixes for units should be printed in roman (upright) type with no space between the prefix and the unit. Compound prefixes should be avoided.

Example: ns but not m μ s for 10^{-9} s

3.3 *Combination of prefixes and symbols*

A combination of prefix and symbol for a unit is regarded as a single symbol which may be raised to a power without the use of brackets.

Examples: cm² means (cm)² and μs^{-1} means (μs)⁻¹

\diamond The superscript $^\circ$ (degree sign) has been widely used with symbols for thermodynamic quantities to denote standard values. It has also been used with other meanings.

3.4 *Multiplication and division of units*

A product of two units may be represented in any of the ways:

$$N\ m\ \text{or}\ N \cdot m\ \text{or}\ N \cdot m\ \text{or}\ N \times m$$

The representation Nm is not recommended.

A quotient of two units may be represented in any of the ways:

$$\frac{m}{s}\ \text{or}\ m/s\ \text{or}\ m\ s^{-1}$$

or in any of the other ways of writing the product of m and s^{-1} .

These rules may be extended to more complex groupings but more than one solidus (/) should never be used in the same expression unless parentheses are used to eliminate ambiguity.

Example: $J \cdot K^{-1} \cdot mol^{-1}$ or $J/(K \cdot mol)$ but never $J/K/mol$

3.5 *The International System of Units (SI units)*

The name International System of Units (SI) has been adopted by the Conférence Générale des Poids et Mesures for the coherent system based on the units: metre, kilogramme, second, ampere, kelvin, and candela. In the International System there is one and only one basic unit for each physical quantity. This is either the appropriate basic SI unit itself (see Section 3.7) or the appropriate derived SI unit formed by multiplication and/or division of two or more basic SI units (see Section 3.10). A few such derived SI units have been given special names and symbols (see Section 3.9).

Decimal fractions and decimal multiples both of the basic and of the derived SI units may, however, be constructed by use of approved prefixes (see Section 3.11).

A seventh unit, the mole, has been recommended for inclusion in the SI by IUPAC but still awaits adoption as such by the Conférence Générale des Poids et Mesures. In this Manual the mole is treated as if it were already part of the SI.

3.6 *Definitions of the basic SI units*

metre: The metre is the length equal to 1 650 763.73 (exactly) wavelengths in a vacuum of the radiation corresponding to the transition between the energy levels $2p_{10}$ and $5d_5$ of the pure nuclide ^{86}Kr .

kilogramme: The kilogramme is the mass of the International Prototype Kilogramme which is in the custody of the Bureau International des Poids et Mesures at Sèvres, France.

second: The second is the duration of 9 192 631 770 periods of the radiation corresponding to the transition between the two hyperfine levels ($F = 4$, $M_F = 0$ and $F = 3$, $M_F = 0$) of the fundamental state ($2S_{\frac{1}{2}}$) of the atom of caesium 133.

ampere: The ampere is that constant current which, if maintained in two parallel rectilinear conductors, of infinite length and of negligible circular cross-section, at a distance apart of 1 metre in a vacuum, would produce a force between the conductors equal to 2×10^{-7} newton per metre of length.

† A coherent system of units is a system based on a selected set of "basic units" from which all "derived units" are obtained by multiplication without introducing numerical factors. In addition there are "dimensionless units", in particular the radian (symbol: rad) for plane angle and the steradian (symbol: sr) for solid angle.

kelvin: The kelvin, unit of thermodynamic temperature, is the fraction $1/273.16$ exactly of the thermodynamic temperature at the triple point of water.

candela: The candela is the luminous intensity, in the perpendicular direction, of a surface of $1/600000$ square metres of a black body at the freezing temperature of platinum under a pressure of 101325 newtons per square metre.

mole: The mole is an amount of substance of a system which contains as many elementary units as there are carbon atoms in 0.012 kg (exactly) of the pure nuclide ^{12}C . The elementary unit *must be specified* and may be an atom, a molecule, an ion, an electron, a photon, etc., or a *specified* group of such entities.

Examples: 1 mole of HgCl has a mass equal to 236.04 grammes
 1 mole of Hg_2Cl_2 has a mass equal to 472.08 grammes
 1 mole of Hg^+ has a mass equal to 200.59 grammes
 1 mole of Hg_2^{2+} has a mass equal to 401.18 grammes
 1 mole of e^- has a mass equal to 5.4860×10^{-4} grammes
 1 mole of a mixture containing 78.09 moles per cent of N_2 , 20.95 moles per cent of O_2 , 0.93 moles per cent of Ar, and 0.03 moles per cent of CO_2 , has a mass equal to 28.964 grammes

3.7 Names and symbols for basic SI units

<i>physical quantity</i>	<i>name of unit</i>	<i>symbol for unit</i>
length	metre	m
mass	kilogramme	kg
time	second	s
electric current	ampere	A
thermodynamic temperature	kelvin	K
luminous intensity	candela	cd
amount of substance	mole	mol

3.8 Names and symbols for supplementary units

These units are dimensionless.

<i>physical quantity</i>	<i>name of unit</i>	<i>symbol for unit</i>
plane angle	radian	rad
solid angle	steradian	sr

3.9 Special names and symbols for derived SI units

<i>physical quantity</i>	<i>name of unit</i>	<i>symbol for unit</i>	<i>definition of unit</i>
force	newton	N	$\text{kg} \cdot \text{m} \cdot \text{s}^{-2}$
energy	joule	J	$\text{kg} \cdot \text{m}^2 \cdot \text{s}^{-2}$
power	watt	W	$\text{kg} \cdot \text{m}^2 \cdot \text{s}^{-3} (= \text{J} \cdot \text{s}^{-1})$
electric charge	coulomb	C	$\text{A} \cdot \text{s}$
electric potential difference	volt	V	$\text{kg} \cdot \text{m}^2 \cdot \text{s}^{-3} \cdot \text{A}^{-1} (= \text{J} \cdot \text{A}^{-1} \cdot \text{s}^{-1})$

◊ In October 1967 the thirteenth Conférence Générale des Poids et Mesures recommended that the kelvin, symbol K, be used both for thermodynamic temperature and for thermodynamic temperature interval, and that the unit-symbols $^{\circ}\text{K}$ and deg be abandoned.

electric resistance	ohm	Ω	$\text{kg} \cdot \text{m}^2 \cdot \text{s}^{-3} \cdot \text{A}^{-2}$ ($= \text{V} \cdot \text{A}^{-1}$)
electric capacitance	farad	F	$\text{A}^2 \cdot \text{s}^4 \cdot \text{kg}^{-1} \cdot \text{m}^{-2}$ ($= \text{A} \cdot \text{s} \cdot \text{V}^{-1}$)
magnetic flux	weber	Wb	$\text{kg} \cdot \text{m}^2 \cdot \text{s}^{-2} \cdot \text{A}^{-1}$ ($= \text{V} \cdot \text{s}$)
inductance	henry	H	$\text{kg} \cdot \text{m}^2 \cdot \text{s}^{-2} \cdot \text{A}^{-2}$ ($= \text{V} \cdot \text{A}^{-1} \cdot \text{s}$)
magnetic flux density	tesla	T	$\text{kg} \cdot \text{s}^{-2} \cdot \text{A}^{-1}$ ($= \text{V} \cdot \text{s} \cdot \text{m}^{-2}$)
luminous flux	lumen	lm	$\text{cd} \cdot \text{sr}$
illumination	lux	lx	$\text{cd} \cdot \text{sr} \cdot \text{m}^{-2}$
frequency	hertz	Hz	s^{-1}

3.10 *Derived SI units and unit-symbols for other quantities*

(This list is not exhaustive.)

<i>physical quantity</i>	<i>SI unit</i>	<i>symbol for SI unit</i>
area	square metre	m^2
volume	cubic metre	m^3
density	kilogramme per cubic metre	$\text{kg} \cdot \text{m}^{-3}$
velocity	metre per second	$\text{m} \cdot \text{s}^{-1}$
angular velocity	radian per second	$\text{rad} \cdot \text{s}^{-1}$
acceleration	metre per second squared	$\text{m} \cdot \text{s}^{-2}$
pressure	newton per square metre	$\text{N} \cdot \text{m}^{-2}$
kinematic viscosity,		
diffusion coefficient	square metre per second	$\text{m}^2 \cdot \text{s}^{-1}$
dynamic viscosity	newton-second	
	per square metre	$\text{N} \cdot \text{s} \cdot \text{m}^{-2}$
electric field strength	volt per metre	$\text{V} \cdot \text{m}^{-1}$
magnetic field strength	ampere per metre	$\text{A} \cdot \text{m}^{-1}$
luminance	candela per square metre	$\text{cd} \cdot \text{m}^{-2}$

3.11 *Prefixes for SI units*

The following prefixes are recommended to indicate decimal fractions or decimal multiples of the basic (Section 3.7) or derived (Section 3.9) SI units.

<i>fraction</i>	<i>prefix</i>	<i>symbol</i>	<i>multiple</i>	<i>prefix</i>	<i>symbol</i>
10^{-1}	deci	d	10	deka	da
10^{-2}	centi	c	10^2	hecto	h
10^{-3}	milli	m	10^3	kilo	k
10^{-6}	micro	μ	10^6	mega	M
10^{-9}	nano	n	10^9	giga	G
10^{-12}	pico	p	10^{12}	tera	T
10^{-15}	femto	f			
10^{-18}	atto	a			

3.12 *Decimal fractions and multiples of SI units having special names*

These units are not part of the SI and their use is to be progressively discouraged. The following list is not exhaustive.

<i>physical quantity</i>	<i>name of unit</i>	<i>symbol for unit</i>	<i>definition of unit</i>
length	ångström	Å	10^{-10} m
length	micron [†]	μ	$10^{-6} \text{ m} = \mu\text{m}$
area	barn	b	10^{-28} m^2

[†] The name micron symbol μ , is still used by some spectroscopists instead of its SI equivalent the micrometre, symbol μm , and likewise the milli-micron, symbol $\text{m}\mu$, instead of the nanometre, symbol nm .

<i>physical quantity</i>	<i>name of unit</i>	<i>symbol for unit</i>	<i>definition of unit</i>
volume	litre [⦿]	l	10^{-3} m^3
mass	tonne	t	10^3 kg
force	dyne	dyn	10^{-5} N
pressure	pascal	Pa	$\text{N} \cdot \text{m}^{-2}$
pressure	bar	bar	$10^5 \text{ N} \cdot \text{m}^{-2}$
energy	erg	erg	10^{-7} J
kinematic viscosity, diffusion coefficient	stokes	St	$10^{-4} \text{ m}^2 \cdot \text{s}^{-1}$
dynamic viscosity	poise	P	$10^{-1} \text{ kg} \cdot \text{m}^{-1} \cdot \text{s}^{-1}$
magnetic flux	maxwell	Mx	10^{-8} Wb
magnetic flux density (magnetic induction)	gauss	G	10^{-4} T
conductance	siemens	S	Ω^{-1}

3.13 *Other units now exactly defined in terms of the SI units*

These units are not part of the SI and their use is to be progressively discouraged. The following list is by no means exhaustive. Each of the definitions given in the fourth column is *exact*.

<i>physical quantity</i>	<i>name of unit</i>	<i>symbol for unit</i>	<i>definition of unit</i>
length	inch	in	$2.54 \times 10^{-2} \text{ m}$
mass	pound (avoirdupois)	lb	0.45359237 kg
force	kilogramme- force	kgf	9.80665 N
pressure	atmosphere	atm	$101325 \text{ N} \cdot \text{m}^{-2}$
pressure	torr	Torr	$(101325/760) \text{ N} \cdot \text{m}^{-2}$
pressure	conventional millimetre of mercury ^{⦿⦿}	mmHg	13.5951×980.665 $\times 10^{-2} \text{ N} \cdot \text{m}^{-2}$
energy	kilowatt-hour	kWh	$3.6 \times 10^6 \text{ J}$
energy	thermo- chemical calorie	cal (thermochem.)	4.184 J
energy	international table calorie	cal _{IT}	4.1868 J

⦿ By decision of the twelfth Conférence Générale des Poids et Mesures in October 1964 the old definition of the litre (1.000028 dm^3) was rescinded. The word litre is now regarded as a special name for the cubic decimetre. Neither the word litre nor its symbol l should be used to express results of high precision.

⦿⦿ The conventional millimetre of mercury, symbol mmHg (not mm Hg), is the pressure exerted by a column exactly 1 mm high of a fluid of density exactly $13.5951 \text{ g} \cdot \text{cm}^{-3}$ in a place where the gravitational acceleration is exactly $980.665 \text{ cm} \cdot \text{s}^{-2}$. The mmHg differs from the Torr by less than $2 \times 10^{-7} \text{ Torr}$.

<i>physical quantity</i>	<i>name of unit</i>	<i>symbol for unit</i>	<i>definition of unit</i>
thermodynamic temperature (<i>T</i>)	degree Rankine [◊]	°R	(5/9) K
customary temperature (<i>t</i>)	degree Celsius [◊]	°C	$t/^{\circ}\text{C} = T/\text{K} - 273.15$
customary temperature (<i>t</i>)	degree Fahren- heit [◊]	°F	$t/^{\circ}\text{F} = T/^{\circ}\text{R} - 459.67$
radioactivity	curie	Ci	$3.7 \times 10^{10} \text{ s}^{-1}$

3.14 *Units defined in terms of the best available experimental values of certain physical constants*

These units are not part of the SI and their use is to be progressively discouraged. The factors for conversion of these units to SI units are subject to change in the light of new experimental measurements of the constants involved. The following list is not exhaustive.

<i>physical quantity</i>	<i>name of unit</i>	<i>symbol for unit</i>	<i>conversion factor</i>
energy	electron-volt	eV	$\text{eV} \approx 1.6021 \times 10^{-19} \text{ J}$
mass	unified atomic mass unit	u	$\text{u} \approx 1.660\,41 \times 10^{-27} \text{ kg}$

3.15 *“International” electrical units*

These units are obsolete having been replaced by the “absolute” (SI) units in 1948. The conversion factors which should be used with electrical measurements quoted in “international” units depend on where and on when the instruments used to make the measurements were calibrated. The following two sets of conversion factors refer respectively to the “mean international” units estimated by the ninth Conférence Générale des Poids et Mesures in 1948, and to the “U.S. international” units estimated by the National Bureau of Standards (U.S.A.) as applying to instruments calibrated by them prior to 1948.

- 1 “mean international ohm” = 1.00049 Ω
- 1 “mean international volt” = 1.00034 V
- 1 “U.S. international ohm” = 1.000495 Ω
- 1 “U.S. international volt” = 1.000330 V

3.16 *Electrical and magnetic units belonging to unit-systems other than the SI*

Definitions of units used in the obsolescent “electrostatic CGS” and “electromagnetic CGS” unit-systems can be found in References 12.1.05 and 12.2.

4. **Numbers**

4.1 *Printing of numbers*

Numbers should be printed in upright type. The decimal sign between digits in a number should be a comma (,) or (but *only* in English-language texts) a point (.). To facilitate the reading of long numbers the digits may be

[◊] The ° sign and the letter following form one symbol and there should be no space between them. Example: 25 °C not 25° C.

grouped in threes but no comma or point should ever be used except for the decimal sign.

Example: 2573,421736 or in English language texts 2573.421736 but never 2,573.421,736

When the decimal sign is placed before the first digit of a number a zero should always be placed before the decimal sign.

Example: 0,2573 $\times 10^4$ or in English language texts 0.2573×10^4 but not ,2573 $\times 10^4$ and not .2573 $\times 10^4$

It is often convenient to print numbers with just one digit before the decimal sign.

Example: 2,573 $\times 10^3$ or in English-language texts 2.573×10^3

4.2 *Multiplication and division of numbers*

The multiplication sign between numbers should be a cross (\times) or (but only in non-English-language texts) a centred dot (\cdot).

Example: 2.3×3.4 or $2,3 \cdot 3,4$

Division of one number by another may be indicated in any of the ways:

$$\frac{136}{273} \quad \text{or} \quad 136/273 \quad \text{or} \quad 136 \times (273)^{-1}$$

These rules may be extended to more complex groupings, but more than one solidus (/) should never be used in the same expression unless parentheses are used to eliminate ambiguity.

Example: $(136/273)/2.303$ or $136/(273 \times 2.303)$ but never $136/273/2.303$

5. **Recommended Mathematical Symbols**[♦]

Mathematical operators (for example d and Δ) and mathematical constants (for example e and π) should always be printed in roman (upright) type.

equal to	=
not equal to	\neq
identically equal to	\equiv
corresponds to	\cong
approximately equal to	\approx
approaches	\rightarrow
asymptotically equal to	\simeq
proportional to	\propto
infinity	∞
smaller than	$<$
larger than	$>$
smaller than or equal to	\leq
larger than or equal to	\geq
much smaller than	\ll
much larger than	\gg
plus	+
minus	-
multiplied by	\cdot \times
a divided by b	$\frac{a}{b}$ a/b ab^{-1}
magnitude of a	$ a $
a raised to the power n	a^n
square root of a	$a^{1/2}$ $a^{\frac{1}{2}}$ \sqrt{a} \sqrt{a}

[♦] Taken from Reference 12.1.11.

n 'th root of a	$a^{1/n}$	$a^{\frac{1}{n}}$	$\sqrt[n]{a}$	$\sqrt[n]{a}$
mean value of a	$\langle a \rangle$	\bar{a}		
natural logarithm of a	$\ln a$	$\log_e a$		
decadic logarithm of a	$\lg a$	$\log_{10} a$		
binary logarithm of a	$\lg a$	$\log_2 a$		
exponential of a	$\exp a$	e^a		

6. Symbols for Chemical Elements, Nuclides, and Particles

6.1 Definitions

A nuclide is a species of atoms of which each atom has identical atomic number (proton number) and identical mass number (nucleon number). Different nuclides that have the same value of the atomic number but different values of the mass number are named isotopes or isotopic nuclides. Different nuclides having the same mass number are named isobars or isobaric nuclides.

6.2 Elements and nuclides

Symbols for chemical elements should be written in roman (upright) type. The symbol is not followed by a full stop except when it occurs at the end of a sentence in text.

Examples: Ca C H He

The attached numerals specify a nuclide:

mass number $^{14}\text{N}_2$ atoms/molecule

The atomic number may be placed in the left subscript position. States of ionization, excitation, or valency may be indicated in the right superscript space.

Examples: Ionized states: Cl^- , SO_4^{2-} , Ca^{2+} , PO_4^{3-}

Excited electronic states: He^* , NO^*

Valence states: $\text{K}_6\text{M}^{\text{IV}}\text{Mo}_9\text{O}_{32}$

6.3 Particles

neutron	n	α -particle	α
proton	p	electron	e
deuteron	d	photon	γ
triton	t		

The electric charge of particles may be indicated by adding the superscript +, -, or °; e.g., p^+ , n^0 , e^+ , e^- . If the symbols p and e are used without charge, they refer to the positive proton and negative electron respectively.

6.4 Abbreviated notation for nuclear reactions

The meaning of the symbolic expression indicating a nuclear reaction should be the following:

initial nuclide (incoming particle(s), or quanta) outgoing particle(s) or quanta final nuclide

Examples: $^{14}\text{N}(\alpha, \text{p})^{17}\text{O}$ $^{59}\text{Co}(\text{n}, \gamma)^{60}\text{Co}$
 $^{23}\text{Na}(\gamma, 3\text{n})^{20}\text{Na}$ $^{31}\text{P}(\gamma, \text{pn})^{29}\text{Si}$

♦ For a more detailed discussion see Reference 12.4.

7. Symbols for Spectroscopy[†]

7.1 General rules

A letter-symbol indicating the quantum state of *a system* should be printed in capital upright type. A letter-symbol indicating the quantum state of *a single particle* should be printed in lower case upright type.

7.2 Atomic spectroscopy

The letter-symbols indicating quantum states are:

$L, l = 0: S, s$	$L, l = 4: G, g$	$L, l = 8: L, l$
$= 1: P, p$	$= 5: H, h$	$= 9: M, m$
$= 2: D, d$	$= 6: I, i$	$= 10: N, n$
$= 3: F, f$	$= 7: K, k$	$= 11: O, o$

A right-hand subscript indicates the total angular momentum quantum number J or j . A left-hand superscript indicates the spin multiplicity $2S+1$.

Examples: ${}^2P_{3/2}$ — state ($J = 3/2$, multiplicity 2)
 $p_{3/2}$ — electron ($j = 3/2$)

An atomic electron configuration is indicated symbolically by:

$$(nl)^{\kappa}(n'l')^{\kappa'} \dots$$

Instead of $l = 0, 1, 2, 3, \dots$ one uses the quantum state symbols s, p, d, f, \dots

Example: the atomic configuration: $(1s)^2(2s)^2(2p)^3$

7.3 Molecular spectroscopy

The letter symbols indicating molecular electronic quantum states are in the case of *linear molecules*:

$$\begin{aligned} \Lambda, \lambda &= 0: \Sigma, \sigma \\ &= 1: \Pi, \pi \\ &= 2: \Delta, \delta \end{aligned}$$

and for *non-linear molecules*:

$$A, a; B, b; E, e; \text{ etc.}$$

Remarks: A left-hand superscript indicates the spin multiplicity. For molecules having a symmetry centre the parity symbol g or u , indicating respectively symmetric or antisymmetric behaviour on inversion, is attached as a right-hand subscript. A $+$ or $-$ sign attached as a right-hand superscript indicates the symmetry as regards reflection in any plane through the symmetry axis of the molecules.

Examples: $\Sigma_g^+, \Pi_u, {}^2\Sigma, {}^3\Pi$, etc.

The letter symbols indicating the vibrational angular momentum states in the case of *linear molecules* are:

$$\begin{aligned} l &= 0: \Sigma \\ &= 1: \Pi \\ &= 2: \Delta \end{aligned}$$

[†] Taken from Reference 12.2.

7.4 Spectroscopic transitions

The upper level and the lower level are indicated by ' and '' respectively.

Examples: $h\nu = E' - E''$ $\sigma = T' - T''$

A spectroscopic transition should be indicated by writing the upper state first and the lower state second, connected by a dash in between.

Examples: ${}^2P_{1/2} - {}^2S_{1/2}$ for an electronic transition
 $(J', K') - (J'', K'')$ for a rotational transition
 $v' - v''$ for a vibrational transition

Absorption transition and emission transition may be indicated by arrows \leftarrow and \rightarrow respectively.

Examples: ${}^2P_{1/2} \rightarrow {}^2S_{1/2}$ emission from ${}^2P_{1/2}$ to ${}^2S_{1/2}$
 $(J', K') \leftarrow (J'', K'')$ absorption from (J'', K'') to (J', K')

The difference Δ between two quantum numbers should be that of the upper state minus that of the lower state.

Example: $\Delta J = J' - J''$

The indications of the branches of the rotation band should be as follows:

$$\begin{aligned}\Delta J = J' - J'' &= -2: \text{O-branch} \\ &= -1: \text{P-branch} \\ &= 0: \text{Q-branch} \\ &= +1: \text{R-branch} \\ &= +2: \text{S-branch}\end{aligned}$$

8. Conventions Concerning the Signs of Electric Potential Differences, Electromotive Forces, and Electrode Potentials[†]

8.1 The electric potential difference for a galvanic cell

The cell should be represented by a diagram, for example:



The electric potential difference ΔV is equal in sign and magnitude to the electric potential of a metallic conducting lead on the right minus that of an identical lead on the left.

When the reaction of the cell is written as:



this implies a diagram so drawn that this reaction takes place when positive electricity flows through the cell from left to right. If this is the direction of the current when the cell is short-circuited, as it will be in the present example (unless the ratio $[\text{Cu}^{2+}]/[\text{Zn}^{2+}]$ is extremely small), the electric potential difference will be positive.

If, however, the reaction is written as:



this implies the diagram



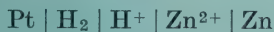
and the electric potential difference of the cell so specified will be negative (unless the ratio $[\text{Cu}^{2+}]/[\text{Zn}^{2+}]$ is extremely small).

[†] The conventions given here are identical with the "Stockholm Convention" of 1953.

The limiting value of the electric potential difference for zero current through the cell is called the electromotive force and denoted by E .

8.2 *Electrode potential*

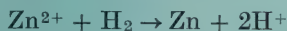
The so-called electrode potential of an electrode (half-cell) is defined as the electromotive force of a cell in which the electrode on the left is a *standard hydrogen electrode* and that on the right is the electrode in question. For example, for the zinc electrode (written as $\text{Zn}^{2+} | \text{Zn}$) the cell in question is:



The reaction taking place at the zinc electrode is:



The latter is to be regarded as an abbreviation for the reaction in the mentioned cell:



In the standard state the electromotive force of this cell has a negative sign and a value of -0.763 V. The standard electrode potential of the zinc electrode is therefore -0.763 V.

The symbol $\text{Zn} | \text{Zn}^{2+}$ on the other hand implies the cell:



in which the reaction is:



The electromotive force of this cell should *not* be called an electrode potential.

9. **The Quantity pH**

9.1 *Operational definition*

In all existing national standards the definition of pH is an operational one. The electromotive force E_X of the cell:

$\text{Pt}, \text{H}_2 | \text{solution X} | \text{concentrated KCl solution} | \text{reference electrode}$ is measured and likewise the electromotive force E_S of the cell:

$\text{Pt}, \text{H}_2 | \text{solution S} | \text{concentrated KCl solution} | \text{reference electrode}$ both cells being at the same temperature throughout and the reference electrodes and bridge solutions being identical in the two cells. The pH of the solution X, denoted by $\text{pH}(\text{X})$, is then related to the pH of the solution S, denoted by $\text{pH}(\text{S})$, by the definition:

$$\text{pH}(\text{X}) = \text{pH}(\text{S}) + \frac{E_X - E_S}{(RT \ln 10)/F}$$

where R denotes the gas constant, T the thermodynamic temperature, and F the Faraday constant. Thus defined the quantity pH is dimensionless.

To a good approximation, the hydrogen electrodes in both cells may be replaced by other hydrogen-ion-responsive electrodes, e.g. glass or quinhydrone. The two bridge solutions may be of any molality not less than $3.5 \text{ mol} \cdot \text{kg}^{-1}$, provided they are the same (see Reference 12.5).

The difference between the pH of two solutions having been defined as above, the definition of pH can be completed by assigning a value of pH at each temperature to one or more chosen solutions designated as standards. A series of pH(S) values for five suitable standard reference solutions is given in 9.3.

If the definition of pH given above is adhered to strictly, then the pH of a solution may be slightly dependent on which standard solution is used. These unavoidable deviations are caused not only by imperfections in the response of the hydrogen-ion electrodes but also by variations in the liquid junctions resulting from the different ionic compositions and mobilities of the several standards and from differences in the geometry of the liquid-liquid boundary. In fact such variations in measured pH are usually too small to be of practical significance. Moreover, the acceptance of several standards allows the use of the following alternative definition of pH.

The electromotive force E_X is measured, and likewise the electromotive forces E_1 and E_2 of two similar cells with the solution X replaced by the standard solutions S_1 and S_2 such that the E_1 and E_2 values are on either side of, and as near as possible to, E_X . The pH of solution X is then obtained by assuming linearity between pH and E , that is to say

$$\frac{\text{pH}(X) - \text{pH}(S_1)}{\text{pH}(S_2) - \text{pH}(S_1)} = \frac{E_X - E_1}{E_2 - E_1}$$

This procedure is especially recommended when the hydrogen-ion-responsive electrode is a glass electrode.

9.3 Values of pH(S) for five standard solutions

$t/^{\circ}\text{C}$	A	B	C	D	E
0		4.003	6.984	7.534	9.464
5		3.999	6.951	7.500	9.395
10		3.998	6.923	7.472	9.332
15		3.999	6.900	7.448	9.276
20		4.002	6.881	7.429	9.225
25	3.557	4.008	6.865	7.413	9.180
30	3.552	4.015	6.853	7.400	9.139
35	3.549	4.024	6.844	7.389	9.102
38	3.548	4.030	6.840	7.384	9.081
40	3.547	4.035	6.838	7.380	9.068
45	3.547	4.047	6.834	7.373	9.038
50	3.549	4.060	6.833	7.367	9.011
55	3.554	4.075	6.834		8.985
60	3.560	4.091	6.836		8.962
70	3.580	4.126	6.845		8.921
80	3.609	4.164	6.859		8.885
90	3.650	4.205	6.877		8.850
95	3.674	4.227	6.886		8.833

The compositions of the standard solutions are:

A: KH tartrate (saturated at 25 $^{\circ}\text{C}$)

B: KH phthalate, $m = 0.05 \text{ mol} \cdot \text{kg}^{-1}$

C: KH_2PO_4 , $m = 0.025 \text{ mol} \cdot \text{kg}^{-1}$;
 Na_2HPO_4 , $m = 0.025 \text{ mol} \cdot \text{kg}^{-1}$

D: KH_2PO_4 , $m = 0.008695 \text{ mol} \cdot \text{kg}^{-1}$;
 Na_2HPO_4 , $m = 0.03043 \text{ mol} \cdot \text{kg}^{-1}$
 E: $\text{Na}_2\text{B}_4\text{O}_7$, $m = 0.01 \text{ mol} \cdot \text{kg}^{-1}$

where m denotes molality.

10. Definition of Rate of Reaction and Related Quantities

10.1 Rate of reaction

For the reaction

$$0 = \sum_{\text{B}} \nu_{\text{B}} \text{B}$$

the extent of reaction ξ is defined according to 2.5.03 by

$$d\xi = \nu_{\text{B}}^{-1} dn_{\text{B}}$$

where n_{B} is the amount, and ν_{B} is the stoichiometric number, of the substance B.

It is recommended that the *rate of reaction* be defined as the rate of increase of the extent of reaction, namely

$$\dot{\xi} = d\xi/dt = \nu_{\text{B}}^{-1} dn_{\text{B}}/dt$$

This definition is independent of the choice of B and is valid regardless of the conditions under which a reaction is carried out, e.g. it is valid for a reaction in which the volume varies with time, or for a reaction involving two or more phases, or for a reaction carried out in a flow reactor.

If both sides of this equation are divided by any specified volume V , not necessarily independent of time, and not necessarily that of a single phase in which the reaction is taking place, then

$$V^{-1} d\xi/dt = V^{-1} \nu_{\text{B}}^{-1} dn_{\text{B}}/dt$$

If the specified volume V is independent of time, then

$$V^{-1} d\xi/dt = \nu_{\text{B}}^{-1} d(n_{\text{B}}/V)/dt$$

If this specified volume V is such that

$$n_{\text{B}}/V = c_{\text{B}} \text{ or } [\text{B}]$$

where c_{B} or $[\text{B}]$ is the concentration of B, then

$$V^{-1} d\xi/dt = \nu_{\text{B}}^{-1} dc_{\text{B}}/dt \text{ or } \nu_{\text{B}}^{-1} d[\text{B}]/dt$$

The quantity

$$dn_{\text{B}}/dt \quad (= \nu_{\text{B}} d\xi/dt)$$

may be called the rate of formation of B, and the quantity

$$V^{-1} \nu_{\text{B}}^{-1} dn_{\text{B}}/dt \quad (= V^{-1} d\xi/dt)$$

may be called the rate of reaction divided by volume, and the quantity

$$v_{\text{B}} = dc_{\text{B}}/dt \text{ or } d[\text{B}]/dt$$

which has often been called the rate of reaction, may be called the rate of increase of the concentration of B, but none of these three quantities should be called the rate of reaction.

10.2 Order of reaction

If it is found *experimentally* that the rate of increase of the concentration of B is given by

$$v_B \propto [C]^c [D]^d \dots$$

then the reaction is described as of order c with respect to C, of order d with respect to D, ..., and of overall order $(c + d + \dots)$.

10.3 Molecularity and elementary processes

Elementary processes are called unimolecular, bimolecular, trimolecular, according to the number of molecules reacting.

They should be labelled in such a manner that reverse processes are immediately recognizable.

<i>Example: elementary process</i>	<i>label</i>	<i>rate constant</i>
$\text{Br}_2 + \text{M} \rightarrow 2\text{Br} + \text{M}$	+ 1	k_{+1}
$\text{Br} + \text{H}_2 \rightarrow \text{HBr} + \text{H}$	+ 2	k_{+2}
$\text{H} + \text{Br}_2 \rightarrow \text{HBr} + \text{Br}$	+ 3	k_{+3}
$\text{H} + \text{HBr} \rightarrow \text{H}_2 + \text{Br}$	- 2	k_{-2}
$2\text{Br} + \text{M} \rightarrow \text{Br}_2 + \text{M}$	- 1	k_{-1}

10.4 Collision number

The collision number defined as the number of collisions per unit time and per unit volume and having dimensions $(\text{time})^{-1} \times (\text{volume})^{-1}$ should be denoted by Z .

The collision number divided by the product of two relevant concentrations (or by the square of the relevant concentration) and by the Avogadro constant is a second-order rate constant having dimensions $(\text{time})^{-1} \times (\text{volume}) \times (\text{amount of substance})^{-1}$ and should be denoted by z . Thus $z = Z/Lc_Ac_B$.

11. Values of the Fundamental Constants

At the XXIIIrd Conference of IUPAC the Council recommended the use by chemists of a consistent set of fundamental constants which has been published (see Reference 12.6). For the details concerning the development of this set of constants and their assigned uncertainties the reader is referred to the original paper and references therein. For convenience the recommended values are given here for the most important quantities.

<i>quantity</i>	<i>symbol</i>	<i>value (with estimated uncertainty)</i>
speed of light	c	$2.997\,925 \times 10^8 \text{ m} \cdot \text{s}^{-1}$
in vacuum		$\pm 0.000\,003 \times 10^8 \text{ m} \cdot \text{s}^{-1}$
Avogadro constant	L, N_A	$6.022\,52 \times 10^{23} \text{ mol}^{-1}$
		$\pm 0.000\,28 \times 10^{23} \text{ mol}^{-1}$
Faraday constant	F	$9.648\,70 \times 10^4 \text{ C} \cdot \text{mol}^{-1}$
		$\pm 0.000\,16 \times 10^4 \text{ C} \cdot \text{mol}^{-1}$
Planck constant	h	$6.625\,6 \times 10^{-34} \text{ J} \cdot \text{s}$
		$\pm 0.000\,5 \times 10^{-34} \text{ J} \cdot \text{s}$
"ice-point"	T_{ice}	$273.150\,0 \text{ K}$
temperature \diamond		$\pm 0.000\,1 \text{ K}$

\diamond The "ice-point" temperature T_{ice} is the temperature of equilibrium of solid and liquid water saturated with air at a pressure of one atmosphere. The quantity RT_{ice} is identical to the quantity $\lim_{p \rightarrow 0} (pV_m)$ for a gas at $T' = T_{\text{ice}} = 273.1500 \text{ K}$.

	RT_{ice}	$2.271\,06 \times 10^3 \text{ J} \cdot \text{mol}^{-1}$
		$\pm 0.000\,12 \times 10^3 \text{ J} \cdot \text{mol}^{-1}$
gas constant	R	$8.314\,33 \text{ J} \cdot \text{K}^{-1} \cdot \text{mol}^{-1}$
		$\pm 0.000\,44 \text{ J} \cdot \text{K}^{-1} \cdot \text{mol}^{-1}$
charge of proton	e	$1.602\,10 \times 10^{-19} \text{ C}$
		$\pm 0.000\,07 \times 10^{-19} \text{ C}$
Boltzmann constant	k	$1.380\,54 \times 10^{-23} \text{ J} \cdot \text{K}^{-1}$
		$\pm 0.000\,09 \times 10^{-23} \text{ J} \cdot \text{K}^{-1}$
second radiation constant	$c_2 = hc/k$	$1.438\,79 \times 10^{-2} \text{ m} \cdot \text{K}$
		$\pm 0.000\,09 \times 10^{-2} \text{ m} \cdot \text{K}$
Einstein constant relating mass and energy	$Y = c^2$	$8.987\,554 \times 10^{16} \text{ J} \cdot \text{kg}^{-1}$
		$\pm 0.000\,018 \times 10^{16} \text{ J} \cdot \text{kg}^{-1}$
constant relating wave-number and energy	$Z = N_A hc$	$1.196\,255 \times 10^{-1} \text{ J} \cdot \text{m} \cdot \text{mol}^{-1}$
		$\pm 0.000\,038 \times 10^{-1} \text{ J} \cdot \text{m} \cdot \text{mol}^{-1}$
Bohr magneton	μ_B	$9.273\,2 \times 10^{-24} \text{ m}^2 \cdot \text{A}$
		$\pm 0.000\,6 \times 10^{-24} \text{ m}^2 \cdot \text{A}$
permeability of vacuum	μ_0	$4\pi \times 10^{-7} \text{ J} \cdot \text{s}^2 \cdot \text{C}^{-2} \cdot \text{m}^{-1}$ (exactly)
permittivity of vacuum	$\epsilon_0 = \mu_0^{-1} c^{-2}$	$8.854\,185 \times 10^{-12} \text{ J}^{-1} \cdot \text{C}^2 \cdot \text{m}^{-1}$
		$\pm 0.000\,018 \times 10^{-12} \text{ J}^{-1} \cdot \text{C}^2 \cdot \text{m}^{-1}$

12. References

- 12.1 ISO Recommendation R 31 will when complete form a comprehensive publication dealing with quantities and units in various fields of science and technology. The following parts have so far been published and can be purchased in any country belonging to ISO from the "Member Body", usually the national standardizing organization of the country.
- 12.1.01 "Part I: Basic quantities and units of the SI", 2nd edition, December 1965.
- 12.1.02 "Part II: Quantities and units of periodic and related phenomena", 1st edition, February 1958.
- 12.1.03 "Part III: Quantities and units of mechanics", 1st edition, December 1960.
- 12.1.04 "Part IV: Quantities and units of heat", 1st edition, December 1960.
- 12.1.05 "Part V: Quantities and units of electricity and magnetism", 1st edition, November 1965.
- 12.1.07 "Part VII: Quantities and units of acoustics", 1st edition, November 1965.
- 12.1.11 "Part XI: Mathematical signs and symbols for use in physical sciences and technology", 1st edition, February 1961.

♦ Parts not yet published are Part 0: General principles concerning quantities, units, and symbols; Part VI: Quantities and units of light and related electromagnetic radiation; Part VIII: Quantities and units of physical chemistry and molecular physics; Part IX: Quantities and units of atomic and nuclear physics; Part X: Quantities and units of nuclear reactions and ionizing radiations; Part XII: Dimensionless parameters.

- 12.2 "Symbols, Units and Nomenclature in Physics", Document UIP 11 (SUN 65-3), published by IUPAP, 1965. This document supersedes Document UIP 9 (SUN 61-44) with the same title, which was published by IUPAP in 1961.
- 12.3 "Manual of Physicochemical Symbols and Terminology", published for IUPAC by Butterworths Scientific Publications, London, 1959. This document was reprinted in the *Journal of the American Chemical Society* (1960) 82, 5517.
- 12.4 "Nomenclature of Inorganic Chemistry", published for IUPAC by Butterworths Scientific Publications, London, 1959. This document was reprinted in the *Journal of the American Chemical Society* (1960) 82, 5523.
- 12.5 *Pure and Applied Chemistry* (1960), 1, 163.
- 12.6 *Pure and Applied Chemistry* (1964), 9, 453.

Appendix I

Definition of Activities and Related Quantities

A.I.1 *Chemical potential and absolute activity*

The chemical potential μ_B of a substance B in a mixture of substances B, C, . . . , is defined by

$$\mu_B = (\partial G / \partial n_B)_{T, p, n_C, \dots}$$

where G is the Gibbs energy of the mixture, T is the thermodynamic temperature, p is the pressure, and n_B, n_C, \dots , are the amounts of the substances B, C, . . . , in the mixture.

(In molecular theory the symbol μ_B is sometimes used for the quantity μ_B/L where L is the Avogadro constant, but this usage is not recommended.)

The absolute activity λ_B of the substance B in the mixture is a dimensionless quantity defined by

$$\lambda_B = \exp(\mu_B/RT) \quad \text{or} \quad \mu_B = RT \ln \lambda_B$$

where R is the gas constant.

The definitions given below often take simpler, though perhaps less familiar, forms when they are expressed in terms of absolute activity rather than in terms of chemical potential. Each of the definitions given below is expressed in both of these ways.

1. Pure substances

A.I.2 *Properties of pure substances*

The superscript \cdot attached to the symbol for a property of a substance denotes the property of the *pure* substance.

A.I.3 *Fugacity of a pure gaseous substance*

The fugacity p^{\bullet} of a pure gaseous substance B is a quantity with the same dimensions as pressure, defined in terms of the absolute activity λ_B^{\bullet} of the pure gaseous substance B by

$$p_B^{\bullet} = \lambda_B^{\bullet} \lim_{p \rightarrow 0} (p/\lambda_B^{\bullet}) \quad (T \text{ const.})$$

or in terms of the chemical potential μ_B by

$$RT \ln p_B^{*\bullet} = \mu_B^\bullet + \lim_{p \rightarrow 0} (RT \ln p - \mu_B^\bullet) \quad (T \text{ const.})$$

where p is the pressure of the gas and T is its thermodynamic temperature. It follows from this definition that

$$\lim_{p \rightarrow 0} (p_B^{*\bullet}/p) = 1 \quad (T \text{ const.})$$

and that

$$RT \ln (p_B^{*\bullet}/p) = \int_0^p (V_B^\bullet - RT/p) dp \quad (T \text{ const.})$$

where V_B^\bullet is the molar volume of the pure gaseous substance B.

A pure gaseous substance B for which $p_B^{*\bullet} = p$ is called a *perfect gas*. It follows that $pV = n_B RT$ for a perfect gas B.

The ratio $(p_B^{*\bullet}/p)$ may be called the fugacity coefficient. The name activity coefficient has sometimes been used for this ratio but is not recommended.

2. Mixtures

A.I.4 Definition of a mixture

The word *mixture* is used to describe a gaseous or liquid or solid phase containing more than one substance, when the substances are all treated in the same way (contrast the use of the word *solution* in Section A.I.9).

A.I.5 Partial pressure

The partial pressure p_B of a substance B in a *gaseous* mixture is a quantity with the same dimensions as pressure defined by

$$p_B = y_B p$$

where y_B is the mole fraction of the substance B in the gaseous mixture and p is the pressure.

A.I.6 Fugacity of a substance in a gaseous mixture

The fugacity p_B^* of the substance B in a gaseous mixture containing mole fractions y_B, y_C, \dots , of the substances B, C, \dots , is a quantity with the same dimensions as pressure, defined in terms of the absolute activity λ_B of the substance B in the gaseous mixture by

$$p_B^* = \lambda_B \lim_{p \rightarrow 0} (y_B p / \lambda_B) \quad (T \text{ const.})$$

or in terms of the chemical potential μ_B by

$$RT \ln p_B^* = \mu_B + \lim_{p \rightarrow 0} \{ RT \ln (y_B p) - \mu_B \} \quad (T \text{ const.})$$

It follows from this definition that

$$\lim_{p \rightarrow 0} (p_B^*/y_B p) = 1 \quad (T \text{ const.})$$

and that

$$RT \ln(p_B^*/y_B p) = \int_0^p (V_B - RT/p) dp \quad (T \text{ const.})$$

where V_B is the partial molar volume (see p.6) of the substance B in the gaseous mixture.

A gaseous mixture of B, C, . . . , for which $p_B^* = y_B p$, $p_C^* = y_C p$, . . . , is called a *perfect gaseous mixture*. It follows that $pV = (n_B + n_C + \dots) RT$ for a perfect gaseous mixture of B, C,

The ratio $(p_B^*/y_B p)$ may be called the fugacity coefficient of the substance B. The name activity coefficient has sometimes been used for this ratio but is not recommended.

When $y_B = 1$ the definitions given in this Section for the fugacity of a substance in a gaseous mixture reduce to those given in Section A.I.3 for the fugacity of a pure gaseous substance.

A.I.7 *Activity coefficient of a substance in a liquid or solid mixture*

The activity coefficient f_B of a substance B in a liquid or solid mixture containing mole fractions x_B, x_C, \dots , of the substances B, C, . . . , is a dimensionless quantity defined in terms of the absolute activity λ_B of the substance B in the mixture by

$$f_B = \lambda_B / \lambda_B^\bullet x_B$$

where λ_B^\bullet is the absolute activity of the pure substance B at the same temperature and pressure, or in terms of the chemical potential μ_B by

$$RT \ln(x_B f_B) = \mu_B - \mu_B^\bullet$$

where μ_B^\bullet is the chemical potential of the pure substance B at the same temperature and pressure.

It follows from this definition that

$$\lim_{x_B \rightarrow 1} f_B = 1 \quad (T, p \text{ const.})$$

A mixture of substances B, C, . . . , for which $f_B = 1, f_C = 1, \dots$, is called an *ideal mixture*.

A.I.8 *Relative activity of a substance in a liquid or solid mixture*

The relative activity a_B of a substance B in a liquid or solid mixture is a dimensionless quantity defined by

$$a_B = \lambda_B / \lambda_B^\bullet$$

or by

$$RT \ln a_B = \mu_B - \mu_B^\bullet$$

where the other symbols are as defined in Section A.I.7.

It follows from this definition that

$$\lim_{x_B \rightarrow 1} a_B = 1 \quad (T, p \text{ const.})$$

A mixture of substances B, C, . . . , for which $a_B = x_B, a_C = x_C, \dots$, is called an *ideal mixture*.

3. Solutions

A.I.9 Definition of a solution

The word *solution* is used to describe a liquid or solid phase containing more than one substance, when for convenience one of the substances, which is called the *solvent*, is treated differently from the other substances, which are called *solutes*. When, as is often but not necessarily the case, the sum of the mole fractions of the solutes is small compared with unity, the solution is called a *dilute solution*. In the following definitions the solvent substance is denoted by A and the solute substances by B, C,

A.I.10 Properties of infinitely dilute solutions

The superscript ∞ attached to the symbol for a property of a solution denotes the property of an *infinitely dilute solution*.

For example if V_B denotes the partial molar volume (see p.6) of the solute substance B in a solution containing molalities m_B, m_C, \dots , or mole fractions x_B, x_C, \dots , of solute substances B, C, . . . , in a solvent substance A, then

$$V_B^\infty = \lim_{\Sigma_B m_B \rightarrow 0} V_B = \lim_{\Sigma_B x_B \rightarrow 0} V_B \quad (T, p \text{ const.})$$

Similarly if V_A denotes the partial molar volume of the *solvent* substance A, then

$$V_A^\infty = \lim_{\Sigma_B m_B \rightarrow 0} V_A = \lim_{\Sigma_B x_B \rightarrow 0} V_A = V_A^\bullet \quad (T, p \text{ const.})$$

where V_A^\bullet is the molar volume of the pure solvent substance A.

A.I.11 Activity coefficient of a solute substance in a solution

The activity coefficient γ_B of a *solute* substance B in a solution (especially in a dilute liquid solution) containing molalities m_B, m_C, \dots , of solute substances B, C, . . . , in a solvent substance A, is a dimensionless quantity defined in terms of the absolute activity λ_B of the solute substance B in the solution by

$$\gamma_B = (\lambda_B/m_B)/(\lambda_B/m_B)^\infty \quad (T, p \text{ const.})$$

or in terms of the chemical potential μ_B by

$$RT \ln(m_B \gamma_B) = \mu_B - (\mu_B - RT \ln m_B)^\infty \quad (T, p \text{ const.})$$

It follows from this definition that

$$\gamma_B^\infty = 1 \quad (T, p \text{ const.})$$

A solution of solute substances B, C, . . . , in a solvent substance A, for which $\gamma_B = 1, \gamma_C = 1, \dots$, is called an *ideal dilute solution*.

The name activity coefficient with the symbol γ_B may be used for the quantity similarly defined but with concentration c_B (see Section 2.3) in place of molality m_B .

Another activity coefficient, called the *rational activity coefficient* of a solute substance B and denoted by $\gamma_{x,B}$ is sometimes used. It is defined in terms of the absolute activity λ_B by

$$\gamma_{x,B} = (\lambda_B/x_B)/(\lambda_B/x_B)^\infty \quad (T, p \text{ const.})$$

or in terms of the chemical potential μ_B by

$$RT \ln (x_B \gamma_{x,B}) = \mu_B - (\mu_B - RT \ln x_B)^\infty \quad (T, p \text{ const.})$$

where x_B is the mole fraction of the solute substance B in the solution. The rational activity coefficient $\gamma_{x,B}$ is related to the (practical) activity coefficient γ_B by the formula:

$$\gamma_{x,B} = \gamma_B (1 + M_A \Sigma_B m_B)$$

A.I.12 *Relative activity of a solute substance in a solution*

The relative activity a_B of a *solute* substance B in a solution (especially in a dilute liquid solution) containing molalities m_B, m_C, \dots , of solute substances B, C, \dots , in a solvent substance A, is a dimensionless quantity defined in terms of the absolute activity λ_B by

$$a_B = (\lambda_B/m^\ominus)/(\lambda_B/m_B)^\infty = m_B \gamma_B / m^\ominus \quad (T, p \text{ const.})$$

or in terms of the chemical potential μ_B by

$$\begin{aligned} RT \ln a_B &= \mu_B - RT \ln m^\ominus - (\mu_B - RT \ln m_B)^\infty \\ &= RT \ln (m_B \gamma_B / m^\ominus) \end{aligned}$$

where m^\ominus is a standard value of molality (usually chosen to be 1 mol kg⁻¹) and where the other symbols are as defined in Section A.I.11.

It follows from this definition of a_B (compare Section A.I.8) that

$$(a_B m^\ominus / m_B)^\infty = 1 \quad (T, p \text{ const.})$$

A solution of solute substances B, C, \dots , in a solvent substance A, for which $a_B = m_B / m^\ominus$, $a_C = m_C / m^\ominus$, \dots , is called an *ideal dilute solution*.

Note: It is regrettable that the name relative activity and the symbol a_B should be used both for the quantity defined in the present Section and for that defined in Section A.I.8 but this usage seems to be firmly established.

The name activity is often used instead of the name relative activity for this quantity.

The name relative activity with the symbol $a_{c,B}$ may be used for the quantity similarly defined but with concentration c_B (see Section 2.3) in place of molality m_B , and a standard value c^\ominus of concentration (usually chosen to be 1 mol dm⁻³) in place of the standard value m^\ominus of molality.

Another relative activity, called the *rational relative activity* of the solute substance B and denoted by $a_{x,B}$, is sometimes used. It is defined in terms of the absolute activity λ_B by

$$a_{x,B} = \lambda_B / (\lambda_B / x_B)^\infty = x_B \gamma_{x,B} \quad (T, p \text{ const.})$$

or in terms of the chemical potential μ_B by

$$\begin{aligned} RT \ln a_{x,B} &= \mu_B - (\mu_B - RT \ln x_B)^\infty \\ &= RT \ln (x_B \gamma_{x,B}) \end{aligned} \quad (T, p \text{ const.})$$

where x_B is the mole fraction of the substance B in the solution. The rational relative activity $a_{x,B}$ is related to the (practical) relative activity a_B by the formula:

$$a_{x,B} = a_B m^\ominus M_A$$

A.I.13 *Osmotic coefficient of the solvent substance in a solution*

The osmotic coefficient g of the *solvent* substance A in a solution (especially in a dilute liquid solution) containing molalities m_B, m_C, \dots , of solute substances B, C, \dots , is a dimensionless quantity defined in terms of the absolute activity λ_A of the solvent substance A in the solution by

$$g = (M_A \Sigma_B m_B)^{-1} \ln(\lambda_A^\bullet / \lambda_A)$$

where λ_A^\bullet is the absolute activity of the pure solvent substance A at the same temperature and pressure, and M_A is the molar mass of the solvent substance A, or in terms of the chemical potential μ_A by

$$g = (\mu_A^\bullet - \mu_A) / RT M_A \Sigma_B m_B$$

where μ_A^\bullet is the chemical potential of the pure solvent substance A at the same temperature and pressure.

For an *ideal dilute solution* as defined in Section A.I.11 or A.I.12 it can be shown that $g = 1$.

Another osmotic coefficient, called the *rational osmotic coefficient* of the solvent substance A and denoted by g_x , is sometimes used. It is defined in terms of the absolute activity λ_A by

$$g_x = \ln(\lambda_A / \lambda_A^\bullet) / \ln x_A = \ln(\lambda_A / \lambda_A^\bullet) / \ln(1 - \Sigma_B x_B)$$

or in terms of the chemical potential μ_A by

$$g_x = (\mu_A - \mu_A^\bullet) / RT \ln x_A = (\mu_A - \mu_A^\bullet) / RT \ln(1 - \Sigma_B x_B)$$

where x_A is the mole fraction of the solvent substance A in the solution. The rational osmotic coefficient g_x is related to the (practical) osmotic coefficient g by the formula:

$$g_x = g M_A \Sigma_B m_B / \ln(1 + M_A \Sigma_B m_B)$$

A.I.14 *Relative activity of the solvent substance in a solution*

The relative activity a_A of the *solvent* substance A in a solution (especially in a dilute liquid solution) containing molalities m_B, m_C, \dots , or mole fractions x_B, x_C, \dots , of solute substances B, C, \dots , is a dimensionless quantity defined in terms of the absolute activity λ_A of the solvent substance A in the solution by

$$a_A = \lambda_A / \lambda_A^\bullet = \exp(-g M_A \Sigma_B m_B) = (1 - \Sigma_B x_B)^{g_x}$$

or in terms of the chemical potential μ_A by

$$RT \ln a_A = \mu_A - \mu_A^\bullet = -RT g M_A \Sigma_B m_B = g_x RT \ln(1 - \Sigma_B x_B)$$

where the other quantities are as defined in Section A.I.13.

Note: The definition in this Section of the relative activity of the *solvent* in a *solution*, is identical with the definition in Section A.I.8 of the relative activity of any substance in a *mixture*. See also the Note in Section A.I.12.

IUPAC-IUB COMMISSION ON BIOCHEMICAL NOMENCLATURE

Tentative Rules

A ONE-LETTER NOTATION FOR AMINO ACID SEQUENCES*

1. *General considerations*

Various difficulties are encountered when presenting the formulas of long protein sequences in the usual three-letter symbols [1]. Space is often at a premium. A one-letter code minimizes this difficulty and has other distinct advantages. In summarizing large amounts of data or in the alignment of homologous protein sequences, it is important that the patterns in the sequences be condensed and simplified as much as possible. Computer techniques are increasingly applied for the storage of sequences of hundreds of amino acid residues and for their evaluation. For this purpose, a one-letter code is the best solution. Finally, a one-letter code is useful in the labeling of individual amino acid side-chains in three-dimensional pictures of protein molecules.

The possibility of using one-letter symbols was mentioned by GAMOW and YČAS [2] in 1958. The idea was systematized by ŠORM *et al.* [3] in 1961. It was used by this group [4–10] and also by FITCH [11] in several papers on the structure of proteins. In extensive compilations of protein structures, ECK and DAYHOFF [12–14] systematically used one-letter symbols derived partly from the code of ŠORM and KEIL. Independent proposals were made by WISWESSER [15] and by BRAUNSTEIN [16].

In view of the increasing number of different notations and the attending problems, the IUPAC-IUB Commission on Biochemical Nomenclature (CBN) has undertaken the task of drafting a single notation for one-letter symbols. The present proposal was evolved by a CBN subcommission (composed of B. KEIL, R. V. ECK, M. O. DAYHOFF and W. E. COHN); it is based principally on the most recent summary published by DAYHOFF and ECK [14].

2. *Limits of application*

In publications, CBN recommends that one-letter symbols be used only in comparisons of long sequences in tables, lists, or figures, and for such special

* Document of the IUPAC-IUB Commission on Biochemical Nomenclature (CBN), approved by CBN in March 1968 and published by permission of the International Union of Pure and Applied Chemistry, the International Union of Biochemistry, and the official publishers to the International Union of Pure and Applied Chemistry, Messrs Butterworths Scientific Publications.

Comments on these Tentative Rules may be sent to any member of CBN: O. HOFFMANN-OSTENHOF (Chairman), W. E. COHN (Secretary), A. E. BRAUNSTEIN, J. S. FRUTON, P. KARLSON, B. KEIL, W. KLYNE, C. LIÉBECQ, E. C. SLATER, E. C. WEBB, or corresponding member, N. TAMIYA.

Reprints of these Tentative Rules may be obtained from WALDO E. COHN, Director, NAS-NRC Office of Biochemical Nomenclature, Oak Ridge National Laboratory, Box Y, Oak Ridge, Tenn. 37830.

use as tagging three-dimensional models of proteins. They should not be used in simple text nor for original reports of experimental details of sequences. This system is not suitable for reporting the details of peptide synthesis, for example, where a fuller description of substituents is needed and where uncommon amino acids may occur. It should not be used in papers where the single-letter system for nucleoside sequences is employed (ref. 1a, sections 5.4 and 5.5), as in representing codons, etc.

3. Principles of the one-letter code

3.1 The letter written at the left-hand end is that of the amino acid residue carrying the free amino group and the letter written at the right-hand end is that of the amino acid residue carrying the free carboxyl group. The absence of punctuation beyond either end of a sequence implies that it is known to be the amino or carboxyl end of the protein. A fragmentary sequence is to be preceded or followed by a slash (/) to indicate that it is not known to be the end of the complete protein (see comment in section 8.2).

3.2 Initial letters are used where there is no ambiguity. There are six such cases: cysteine, histidine, isoleucine, methionine, serine and valine. All the other amino acids share the initial letters A, G, L, P or T and assignments of them must therefore be somewhat arbitrary. These letters are assigned to the most frequently occurring and structurally most simple amino acids. On this basis, the letters A, G, L, P and T are assigned to alanine, glycine, leucine, proline and threonine, respectively.

3.3 The assignment of the other abbreviations is more arbitrary. However, certain clues are helpful. Two are phonetically suggestive, F for *phenylalanine*, and R for *arginine*. For tryptophan, the double ring in the molecule is associated with bulky letter W. The letters N and Q are assigned to asparagine and glutamine, respectively; D and E are assigned to aspartic acid and glutamic acid, respectively. This leaves lysine and tyrosine, to which K and Y are assigned. These are chosen rather than any of the few other remaining letters because they are alphabetically nearest the initial letters L and T. U and O are avoided because U is easily confused with V in handwritten work and O is confused with G, Q, C and D in imperfect computer print-outs and also with zero. J is avoided for linguistic reasons.

3.4 Two other abbreviations are necessary in order to avoid ambiguity. B is assigned to aspartic acid or asparagine when this distinction has not been determined. Z is assigned when glutamic acid and glutamine have not been distinguished. X means that the identity of an amino acid is undetermined, or the amino acid is atypical.

4. Abbreviations, in alphabetical orders

<i>Amino acid</i>		<i>Abbreviation</i>
Alanine	A	A Ala
Arginine	R	B Asx*
Asparagine	N	C Cys
Aspartic acid	D > B*	D Asp
Cysteine	C	E Glu
		F Phe
Glutamine	Q	G Gly
Glutamic acid	E > Z**	H His
Glycine	G	I Ile
Histidine	H	

<i>Amino acid</i>		<i>Abbreviation</i>	
Isoleucine	I	K	Lys ^{''}
		L	Leu
		M	Met
Leucine	L	N	Asn (← Asn)
Lysine	K		
Methionine	M		
Phenylalanine	F	P	Pro
Proline	P	Q	Gln
		R	Arg
Serine	S	S	Ser
Threonine	T	T	Thr
Tryptophan	W		
Tyrosine	Y	V	Val
Valine	V	W	Trp
		X	Unknown or "other"
Unknown or "other"	X	Y	Tyr
		Z	Glx ^{**}

* For Asp or Asn (i.e., for Asx)

** For Glu or Gln (i.e., for Glx)

5. *Spacing*

A very important use of the one-letter notation is in presenting alignments of many homologous sequences. In printing, it often happens that the alignment is not perfectly maintained because of the variable size of the letters and the variable amount of punctuation. This effect can be very troublesome in extensive comparisons. Therefore, **a single typewriter space is left between letters, either as a blank or occupied by punctuation** (see sections 6, 7, 8). The alignment is preserved by allowing exactly the same spacing for each letter, each blank and each punctuation mark, as in typewritten material or, if printed, as in "typewriter type font".

6. *Known and unknown sequences*

A **blank** between letters indicates that the sequence is **known** (see also comment in section 8.2). As in the three letter notation, **parentheses and commas** are used to indicate regions in which the sequence is **unknown** or **undetermined**.

Example (Beta Corticotropin Releasing Factor [17])

In three-letter symbols:

Ser-Tyr-Cys-Phe-His (Asn,Gln)Cys(Pro,Val)Lys-Gly

In one-letter symbols:

S Y C F H(N, Q)C(P, V)K G

7. *Juxtaposition of unknown sequences known to be connected*

Consider the two sequences, one completely known, the other containing peptides of unknown internal sequence.

(a) Ala-Cys-Asp-Glu-Phe-Gly-His-Ile-Lys-Leu-Met-Asn-Pro-Gln

(b) (Ala,Cys,Asp)(Arg,Ser)(Gly,His,Ile)Lys-Leu-Met-Asn-Pro-Gln

In one-letter notation, these become:

(a) A C D E F G H I K L M N P Q

(b) (A, C, D)(R, S)(G, H, I)M L M N P Q

↑ ↑

In the second illustration, two punctuation marks have been crowded into each of two single spaces (indicated by the arrows). In a computer printout, this would not be possible. A single one-space symbol must be used. Here \equiv is used for \equiv to indicate the end of one unknown sequence and the beginning of another, as shown below.

(a) A C D E F G H I K L M N P Q

(b) (A, C, D=R, S=G, H, I) M L M N P Q
 $\uparrow \quad \uparrow$

8. *Juxtaposition of residues inferred, but not known, to be connected*

Consider the following case in which peptides from a second sequence (d) can be aligned with a known, related sequence (c).

(c) A C D E F G H I K L M N P Q

(d) (A.C.D=R, S=G.H.I) K L/M N/P Q/

8.1 In this illustration, the sequences of two of the fragments (A.C.D and G.H.I in (d)), while not determined, are **inferred** with good confidence, which is indicated by **dots** instead of commas between their residues. Where such inferences **cannot** be made with confidence, commas, which retain their original connotation of "unknown sequence" (section 6), should be used, as in the R, S dipeptide.

8.2 The two **internal slashes (/)** separate adjacent amino acids that come from **different peptides not proven experimentally to be connected**. The third (end) slash indicates that Q is not experimentally proven to be at the carboxyl end of the protein, although it is at the carboxyl end of the P-Q dipeptidyl residue.

Comment. The absence of punctuation at the beginning or end of a complete polypeptide or protein sequence indicates the known amino or carboxyl terminal, respectively (see section 3.1).

8.3 Depending on the experimental details and the nature of the inferences to be represented, even more elaborate punctuation may sometimes be required. It is essential, however, that **only one character (or a blank space of similar size) appear between the single letters** to preserve the spacing that is essential for comparisons (see section 5).

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Appendix

Previous Tentative Rules and Proposals of the IUPAC-IUB Commission on Biochemical Nomenclature, all available from the Office of Biochemical Nomenclature (see footnote on p.46), are:

1. Abbreviations and Symbols for Chemical Names of Special Interest in Biological Chemistry
2. Abbreviated Designation of Amino Acid Derivatives and Polypeptides
3. Naming Synthetic Modifications of Natural Peptides
4. Abbreviated Nomenclature of Synthetic Polypeptides (Polymerized Amino Acids)
5. Nomenclature of Vitamins, Coenzymes and Related Compounds: Isoprenoidal Quinones, Folic Acids, Corrinoids, Miscellaneous Compounds
6. Proposals for the Nomenclature of Lipids

**INTERNATIONAL UNION OF PURE AND APPLIED
CHEMISTRY (IUPAC) AND INTERNATIONAL UNION
OF BIOCHEMISTRY (IUB)**

**TENTATIVE RULES FOR CYCLITOL
NOMENCLATURE***

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A. INTRODUCTION

1. Authority

These Rules are issued jointly by the Commission on the Nomenclature of Organic Chemistry¹ of the International Union of Pure and Applied Chemistry (IUPAC) and by the IUPAC/IUB Commission on Biochemical Nomenclature² on the basis of a report by a Joint Cyclitol Nomenclature Subcommittee³.

2. Scope of Cyclitol Nomenclature

Cyclitols are cycloalkanes containing one hydroxyl group on each of three or more ring atoms**. These compounds, and others closely related to them, possess features of relative and absolute stereochemistry that are characteristic of their class and have been extensively studied; but these features are

* These Rules shall be known as the IUPAC/IUB Tentative Cyclitol Nomenclature Rules. Comments should be sent to Prof. P. E. VERKADE, 's-Gravenhage, Ary Schefferstraat 217, Netherlands, or to Prof. O. HOFFMANN-OSTENHOF, Lehrkanzel für Biochemie der Universität Wien, 1090 Vienna, Währinger Strasse 38, Austria.

** Cycloalkanes containing less than three hydroxyl groups are better named by the more general methods of organic chemical nomenclature.

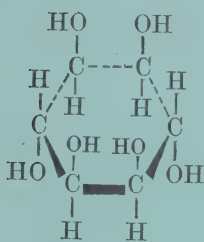
not clearly displayed by general methods of stereochemical nomenclature, so that special methods of specifying their stereochemistry are justified and have long been used. In other than stereochemical respects, their nomenclature should follow the general rules of organic chemistry.

The sequence rule (*R*, *S*) system⁴ may be used when it is desired to relate a cyclitol to the general stereochemical notation and for describing the stereochemistry of chiral groups such as benzylidene which may be present as substituents; but the procedures described below are recommended for cyclitol chemistry as such because of the complexity of the sequence-rule procedure in this field.

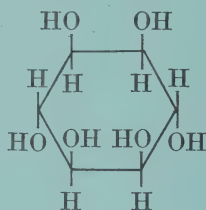
The nomenclature described below is most useful for cycloalkanes containing only one kind of substituent, and specifically for cyclitols and their esters and ethers, but it may also be applied to their derivatives in which one or more hydroxyl groups have been replaced by other groups. It can also be used with advantage for certain cycloalkane derivatives not containing hydroxyl groups, such as polyhalocycloalkanes. No attempt is made here to define the limits of application rigidly.

3. Evolution of Cyclitol Nomenclature

The typical stereochemical feature of cyclitols is exemplified by formula (A), usually drawn more simply as (B) or (C), in which the ring is considered as being planar and perpendicular to the plane of the paper, with hydrogen



(A)



(B)



(C) (Vertical lines denote bonds to OH)

atoms and hydroxyl groups above or below the plane of the ring. In 1900, L. MAQUENNE⁵ devised a fractional notation whereby numerals in the numerator denote hydroxyl or other groups (not hydrogen) above the plane of the ring whilst numerals in the denominator denote hydroxyl or other groups (not hydrogen) below that plane. Thus the above compound received a stereochemical prefix $\frac{1, 2, 4, 5}{3, 6}$ -, which may be more conveniently printed as 1, 2, 4, 5/3, 6-.

MAQUENNE did not, however, lay down exactly how the numerals were to be assigned to the individual positions, and as the chemistry of cyclitols developed so, these assignments were made in different ways. Most notably, logical and self-consistent methods were fully developed (but not assembled as a set of rules) by TH. POSTERNAK⁶, and his methods have been widely used, though with occasional variants, by others. The variety of names that resulted is illustrated in Table I (page 53), which gives also the names derived by the two methods detailed in the Rules below.

Table I Examples of cyclitols named by different systems

R-R: Recommended Rules

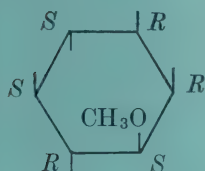
STP: Standardized Traditional Procedure

P: TH. POSTERNAK, ref. 6, where different from STP

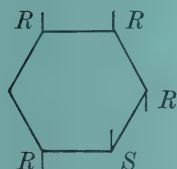
FAL: FLETCHER, ANDERSON, and LARDY, *J.Org.Chem.*, 16, 1238 (1951)

AG: ANGAL and GILHAM, *J.Chem.Soc.*, 1957, 3691

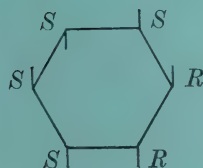
R, S are the sequence rule symbols (ref. 4)



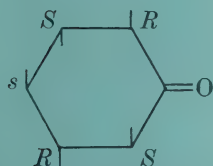
R-R: 1-*O*-Methyl-*myo*-inositol
STP: 3-*O*-Methylmyoinositol
FAL: L-1-*O*-Methyl-*myo*-inositol
AG: (1*S*)-1-*O*-Methyl-*myo*-inositol
Trivial name: (—)-Bornesitol



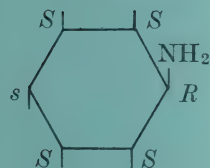
R-R: 1, 2, 4/3, 5-Cyclohexanepentol
STP: 1, 2, 4/3, 5-Cyclohexanepentol
FAL: D-1-Deoxy-*myo*-inositol
AG: (1*R*)-*vibo*-Quercitol
Trivial name: (—)-Viburnitol



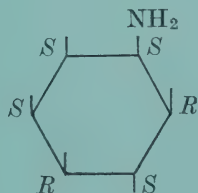
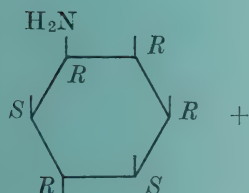
R-R: D-*chiro*-Inositol
STP: (+)-Chiroinositol, 1, 2, 5/3, 4, 6-inositol
FAL: D-Inositol
AG: (1*S*)-Inositol, (1*S*)-1, 2, 4/3, 5, 6-inositol



R-R: 2, 4, 6/3, 5-Pentahydroxycyclohexanone
STP: 2, 4, 6/3, 5-Pentahydroxycyclohexanone
P: Scyllomesoinosose, mesoinosose-2
FAL: *myo*-Inosose-2
AG: *scyllo*-Inosose

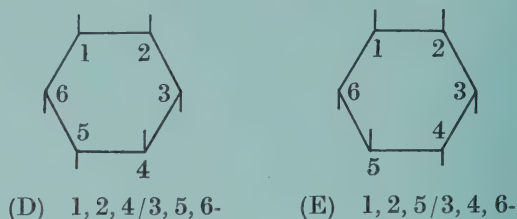


R-R: 1-Amino-1-deoxy-*neo*-inositol
STP: 1, 2, 3*N*/4, 5, 6-Inosamine
P: Neoinosamine-3
FAL: L-*neo*-Inosamine-1
AG: (1*S*)-1-Amino-1-deoxy-*neo*-inositol



R-R: DL-2-Amino-2-deoxy-*epi*-inositol
STP: (±)-2(4)-Amino-2(4)-deoxyepiinositol
FAL: DL-*epi*-Inosamine-2
AG: (±)-2-Amino-2-deoxy-*epi*-inositol

It is an advantage of the Posternak system that the resulting fractional prefix describes, not only the relative positions of the substituents, but also the absolute configuration of a compound: no additional prefix such as D or L or *R* or *S* is needed to differentiate enantiomers, since pairs of enantiomers receive different fractional prefixes by this system, e.g. the enantiomers (D) and (E):



This very feature, however, entails serious disadvantages. The fractional prefix—which is all that may be used—gives no indication whether a compound so specified is chiral or achiral, and for a pair of enantiomers gives no indication that they have the same relative stereochemistry, i.e. that they are enantiomers. This is contrary to the practice in the rest of chemical literature, whereby enantiomers receive identical names except for a specific prefix denoting the chirality. Also specification of racemates becomes somewhat cumbersome by this system in certain cases.

An alternative method of assigning numerals, based in part on previous practice, was elaborated by S.J. ANGYAL and L. ANDERSON in conjunction with the remainder of the Joint Cyclitol Nomenclature Sub-Committee. By this method, enantiomers receive identical fractional prefixes that specify relative stereochemistry, but they receive also an additional prefix D or L (DL is used for a racemate) which specifies the chirality (absolute stereochemistry).

By a majority, the Joint Cyclitol Nomenclature Sub-Committee recommended the latter procedure and this is adopted by the parent IUPAC and IUB Nomenclature Commissions mentioned above. It is defined below in Part B, headed "Recommended Rules".

At the same time it has seemed advisable to set out detailed Rules for the older system, because it has been so widely used in cyclitol literature hitherto, and also so that those continuing to use it may avoid variants by referring to the procedures here assembled for the first time. These non-preferred Rules are, therefore, given in Part C under the title "Standardized Traditional Procedure"; they are based on the methods used in TH. POSTERNAK'S book⁶.

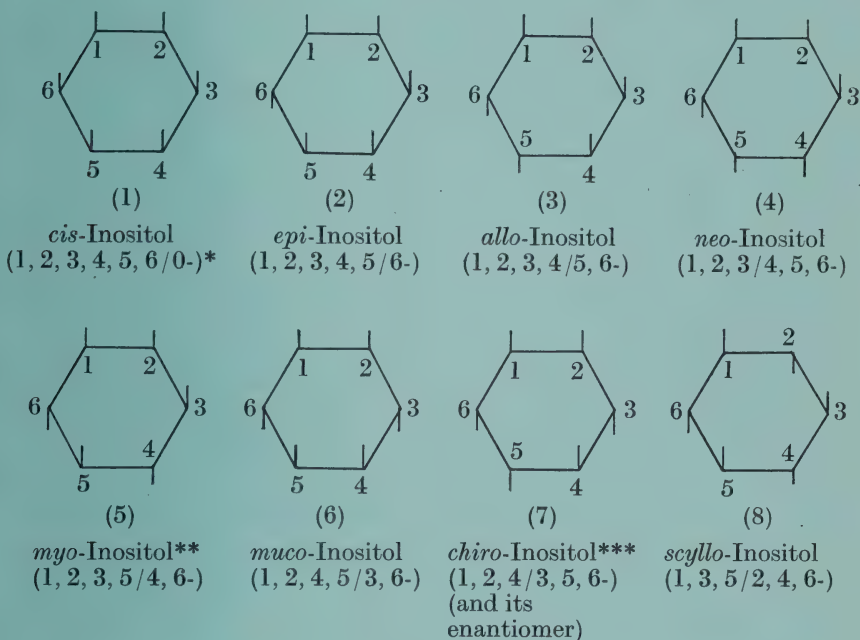
To aid comparison, the same examples are, in general, used for both sets of Rules, with the same identifying reference numerals.

B. RECOMMENDED RULES

Rule I-1 *Trivial names*

[1- (for Inositol) is attached to the Rule numbers as a general identifying prefix.]

I-1.1 1, 2, 3, 4, 5, 6-Cyclohexanehexols are termed generically "inositols". Individual inositols are differentiated by use of an italicized prefix and hyphen, as follows, the locants (positional numbers) being assigned as described in Rule I-3:



These prefixes are used also for inositol derivatives that contain at least three hydroxyl groups or substituted hydroxyl groups; the fractional notation (see below) is used instead for inositol derivatives containing less than three such groups.

I-1.2 *x*-Amino-*x*-deoxyinositols are termed generically "inosamines"; 2, 3, 4, 5, 6-pentahydroxy-1-cyclohexanones are termed generically "ino-

*Preferred to "all-*cis*-" in this and similar cases. The zero is inserted for clarity.

***myo*-Inositol is preferred to *meso*-inositol (which has also been used), because *myo* defines the single configuration 1, 2, 3, 5/4, 6-, whereas *meso* has general significance.

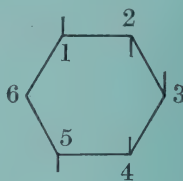
***Replaces "inositol". Some form of chirality symbol is also required. The prefix *chiro* denotes that these are the only unsubstituted inositols that exist in enantiomeric (chiral) forms.

sores". Individual members of these series are preferably named according to the Rules set out below.

I-1.3 The trivial name (–)-quinic acid is preferred for the compound illustrated (cf. Example (45), page 67). The trivial name (+)-quercitol is permitted for (1L)-1, 3, 4/2, 5-cyclohexanepentol (for derivation of this name see below). The generic name "quercitols" is abandoned.



(–)-Quinic acid



(+)-Quercitol

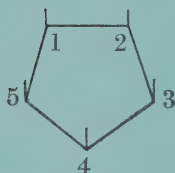
Rule I-2 *Relative configuration*

I-2.1 The relative configurations at ring positions of a cyclitol, other than an inositol or a derivative thereof, are described by means of a fraction which, together with a hyphen, is placed in front of the complete name of the compound, except that *O*-substituents precede the fraction. The numerator consists of the locants (positional numbers, assigned as described below) of those substituents (called below a "set") that lie above or below the plane of the ring, these numbers being arranged in ascending order and separated by commas. The denominator contains the locants of the other set. Conventionally, the set of locants containing the lowest numbers is cited as numerator.

Notes: (1) The fraction may be written with a horizontal or a sloping division line, e.g. $\frac{1, 2, 4}{3, 5, 6}$ or 1, 2, 4/3, 5, 6-.

- (2) "Lowest numbers" are those that, when considered as a single ascending series, contain the lower number at the first point of difference; e.g. 1, 2, 3, 6 is lower than 1, 2, 4, 5.
- (3) This system of nomenclature differs from the system described in Part C in that it is only conventional which set of locants forms the numerator of the fraction.
- (4) The special position of *O*-substituents is illustrated in example (35), page 76.

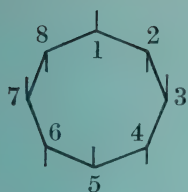
Examples:*



1, 2, 3, 4, 5/0-Cyclopentanepentol

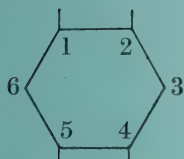
(9)

*Throughout these Examples a simple vertical stroke signifies a bond to a hydroxyl group (cf. p. 52).



1, 3, 5, 7/2, 4, 6, 8-Cyclooctaneoctol

(10)



1, 2/4, 5-Cyclohexanetetrol

(11)

Rule I-3 *Assignment of locants (positional numbers to cyclitols containing only hydroxyl or substituted hydroxyl groups*

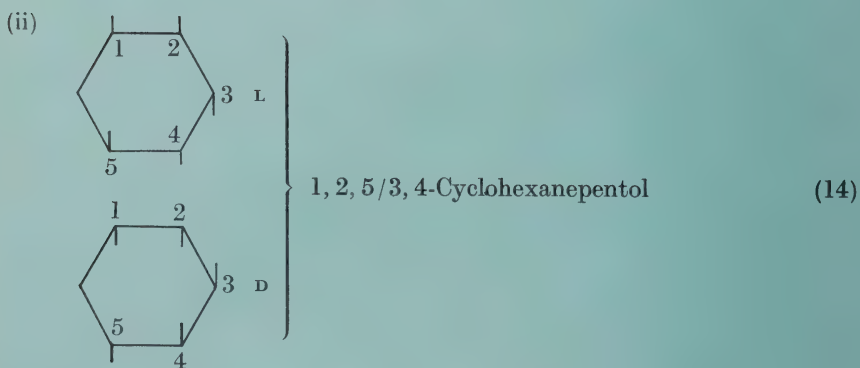
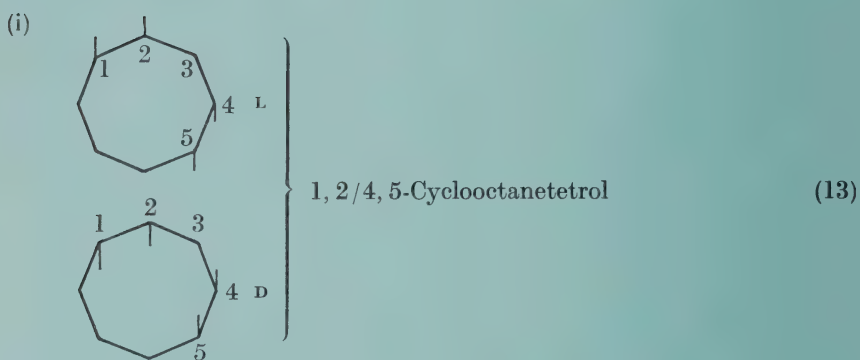
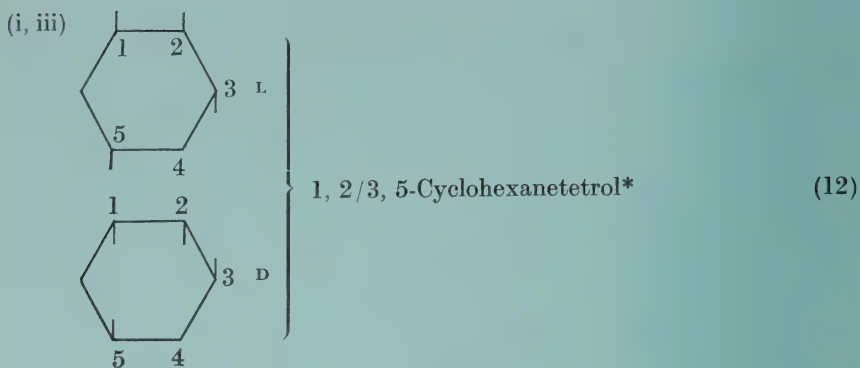
I-3.1. Locants (positional numbers) are assigned to the carbon atoms of the ring, and thus the direction of numbering is described, with reference to the steric relations and nature of the substituents attached to the ring. Lowest locants are related to one set of the substituents according to the following criteria, which are applied successively until a decision is reached:

- (i) to the substituents considered as a numerical series, without regard to configuration;
- (ii) if one set of substituents is more numerous than the other, to the more numerous;
- (iii) if the sets are equally numerous and one of them can be denoted by lower numbers, to that set;
- (iv) to substituents other than unmodified hydroxyl groups;
- (v) to the substituent first in alphabetical order (*Chemical Abstracts*)⁷ or of less complexity (BEILSTEIN's *Handbuch der organischen Chemie*)⁸;
- (vi) (for *meso*-compounds only) to those positions that lead to an L-rather than a D-designation when Rule I-5 is applied to the lowest-numbered asymmetric carbon atom.

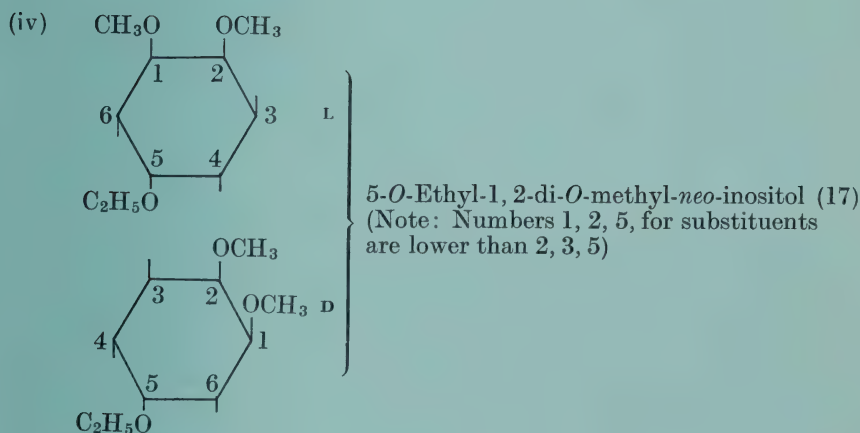
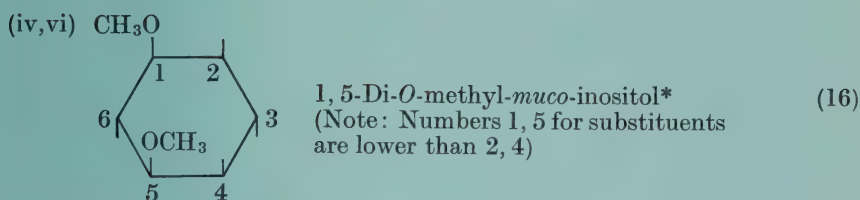
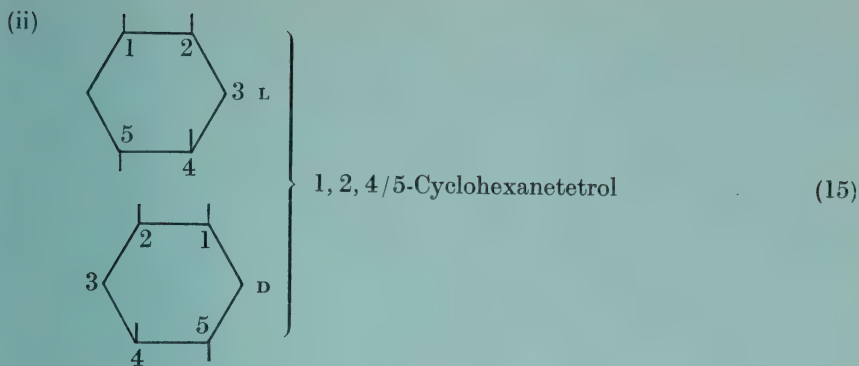
For inositols, criteria (iv) and (v) are applied only when the numbering illustrated in Rule I-1 is not thereby altered.

- Notes:*
- (1) In conformity with other IUPAC Rules, the alphabetical order of prefixes is used in these Rules, except that both names are given when criterion (v) operates.
 - (2) Criterion (vi) is needed only for compounds with *meso*-configuration, being required only for problems involving prochirality⁹. It can be simply applied by noting that it causes numbering to be clockwise when the formula is oriented so that the substituent on the lowest-numbered asymmetric carbon atom of the ring projects upwards.
 - (3) In some cases, for example (7), (9), (10), and (11), various positions are fully equivalent and it is then immaterial which of the equivalent starting points is chosen.

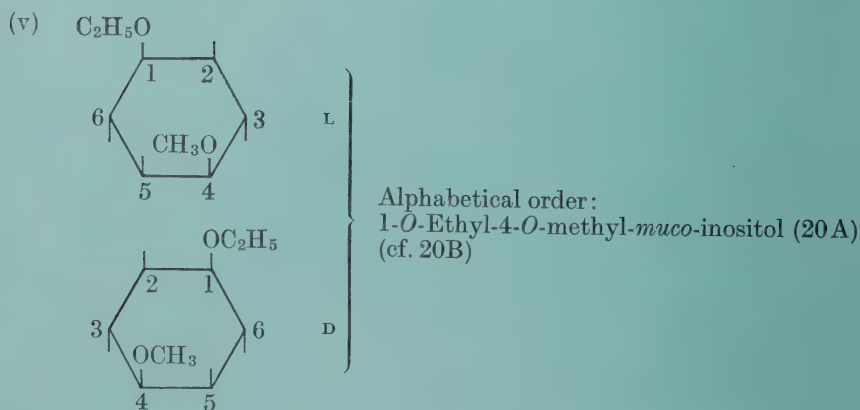
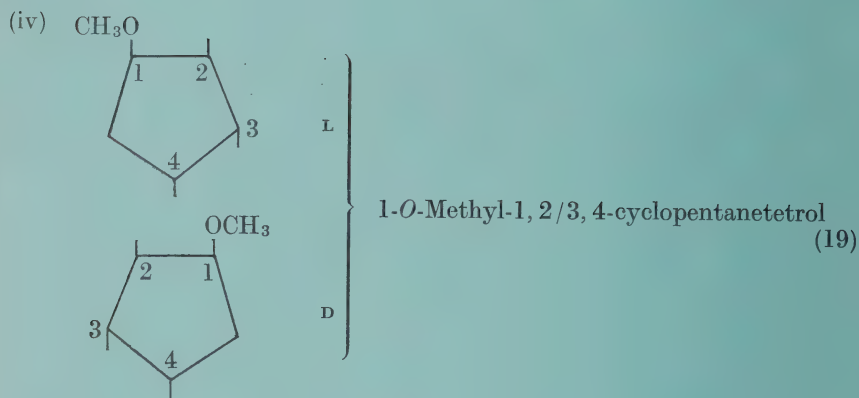
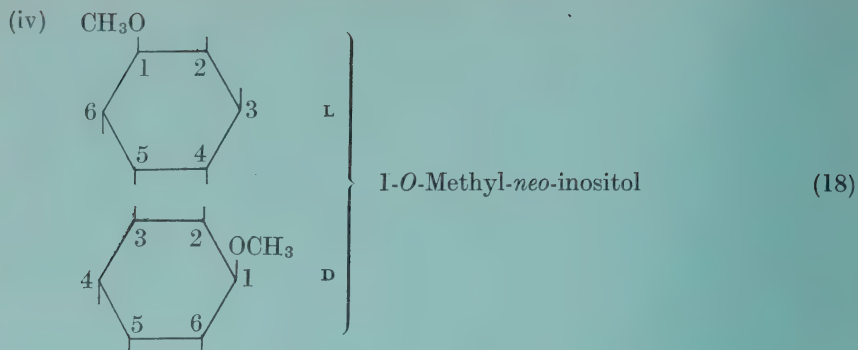
Examples:

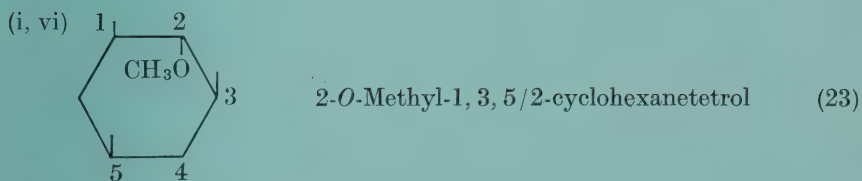
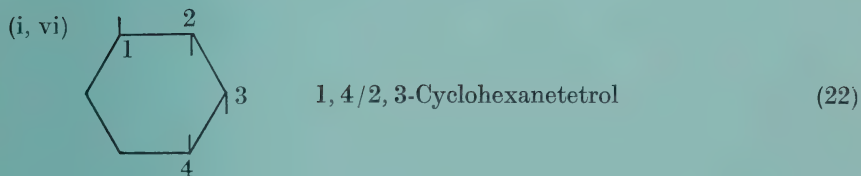
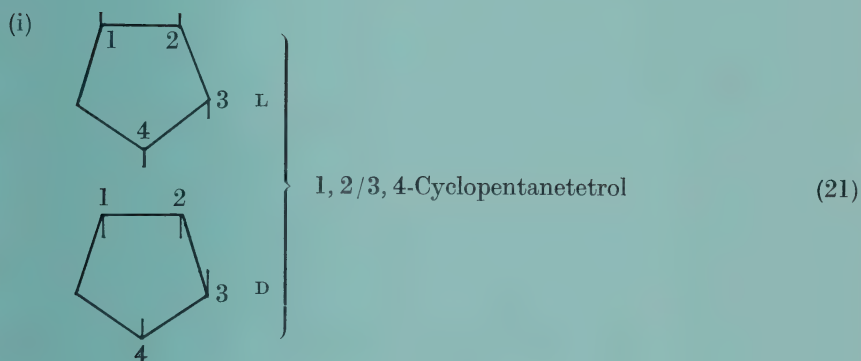
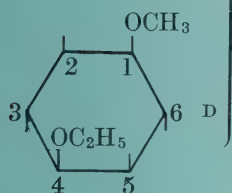
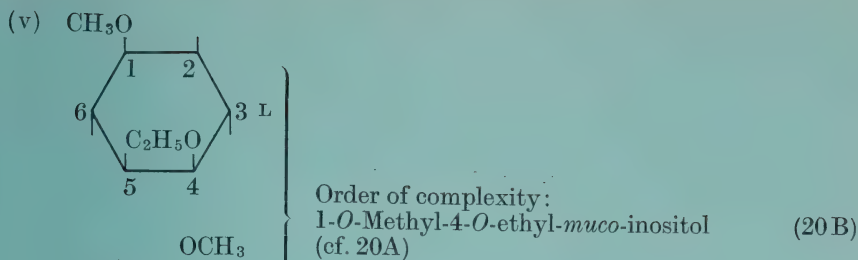


*For allocation of D and L to these and other enantiomers in the Examples see Rule I-5.

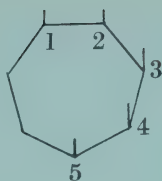


*As exceptions to general nomenclature but in accord with carbohydrate nomenclature, ethers and esters of cyclitols may be named by using prefixes such as 1-*O*-methyl, 1-*O*-acetyl, etc., or by adding 1-methyl ether, 1-acetate, etc., after the name of the polyol. For simplicity only the former alternative is used in these Examples.





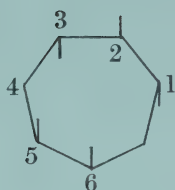
(i, vi)



1, 2, 3, 4, 5/0-Cycloheptanepentol

(24)

(i, vi)

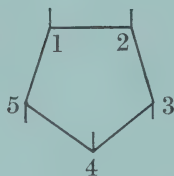


1, 3/2, 5, 6-Cycloheptanepentol

(25)

(i, vi) See also Example (11)

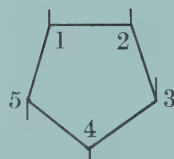
(ii, vi)



1, 2, 4/3, 5-Cyclopentanepentol

(26)

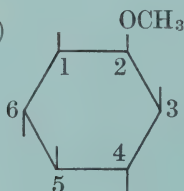
(ii, vi)



1, 2, 3/4, 5-Cyclopentanepentol

(27)

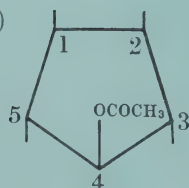
(ii, vi)



2-*O*-Methyl-*myo*-inositol

(28)

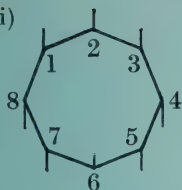
(ii, vi)



4-*O*-Acetyl-1, 2, 4/3, 5-Cyclopentanepentol

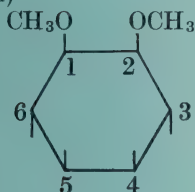
(29)

(iii, vi)



1, 2, 3, 6/4, 5, 7, 8-Cyclooctaneoctol (30)

(iv, vi)



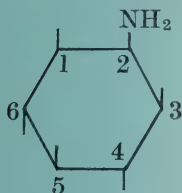
1, 2-Di-O-methyl-muco-inositol (31)

(ii, vi) See also Examples (2), (3), (5), and (6)

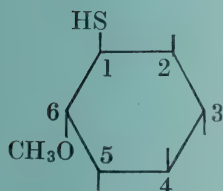
Rule I-4 *Assignment of locants (positional numbers) to cyclitols containing substituents other than hydroxyl or modified hydroxyl groups*

I-4.1 If one or two hydroxyl groups of an inositol are replaced by other univalent substituents with retention of configuration, and if, according to the IUPAC 1965 Rules for Nomenclature of Organic Chemistry, Section C, these substituents do not require to be named as suffixes, then the configurational prefix and the numbering of the parent inositol are retained and "deoxy" nomenclature is used. (For cyclitols the most important part of the order of decreasing priority for citation as suffix is: COOH and modified COOH, =O, OH, SH, NH₂.)

Examples:

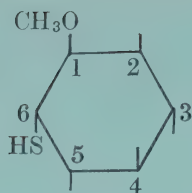


2-Amino-2-deoxy-myo-inositol (32)



Alphabetical order:
1L-1-Deoxy-1-mercapto-6-O-methyl-chiro-inositol* (33A)
(cf. 33B)

* See footnote on p. 64.



Order of complexity:

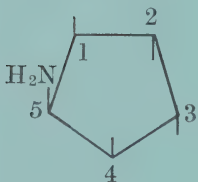
1L-1-*O*-Methyl-6-mercapto-6-deoxy-
chiro-inositol*
(cf. 33A)

(33B)

I-4.2 Cyclitols containing substituents other than hydroxyl or modified hydroxyl (excepting inositols covered by Rule I-4.1) are named and numbered according to the above-mentioned IUPAC Rules. When this leaves alternatives available, the criteria (ii) to (vi) of Rule I-3 are applied. When the substituent is a univalent group the fraction describing the configuration is placed in parentheses in front of the complete name.

Note: The IUPAC Rule C-10 provides that one type of group be chosen as suffix, named as suffix, and given the lowest possible number(s), the remaining types being named as prefixes. For choice of suffix see the last (parenthetical) sentence in Rule I-4.1.

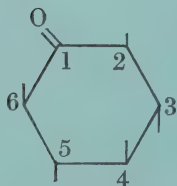
Examples:



(1,4,5/2,3)-5-Amino-1,2,3,4-cyclopentanetetrol
(34)

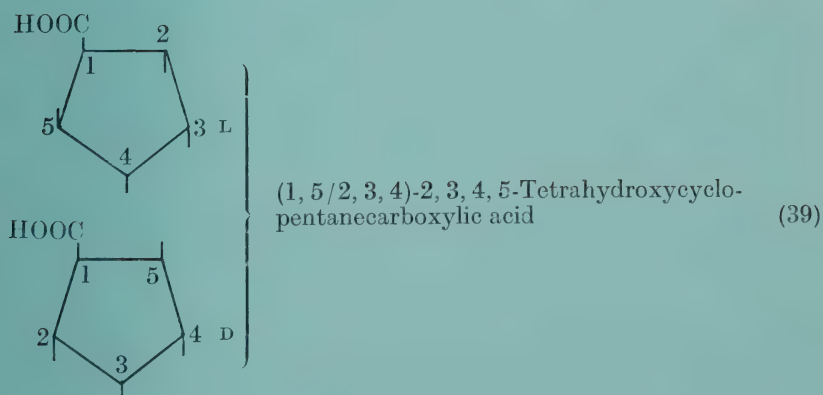
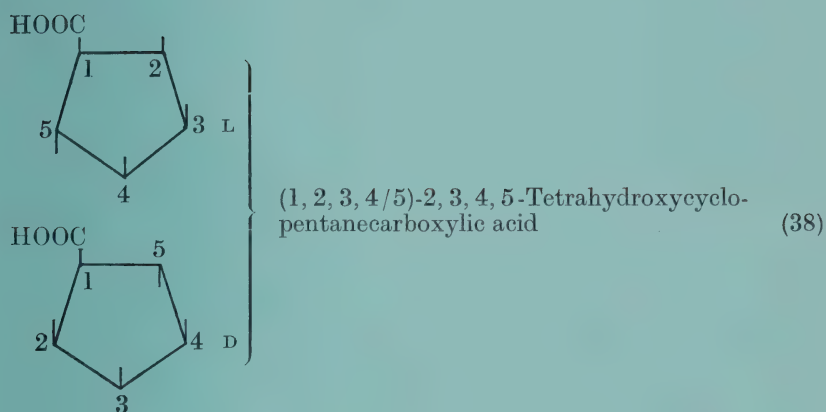
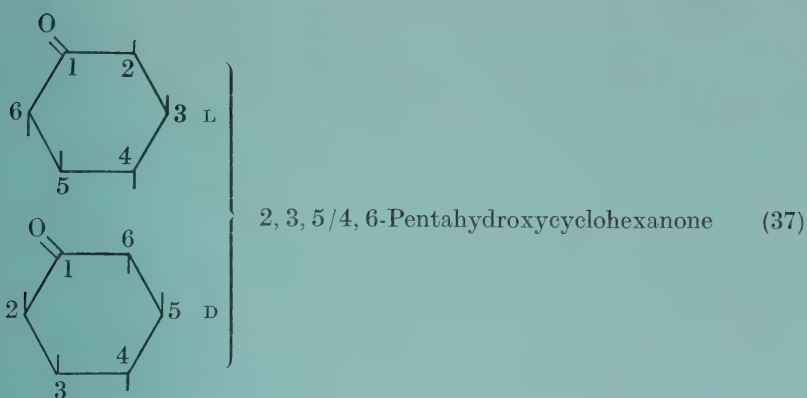


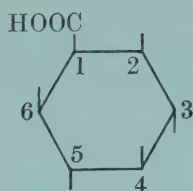
1D-1-*O*-Methyl-(1,2/4,5)-4-Amino-
5-mercapto-1,2-cyclohexanediol
(35)



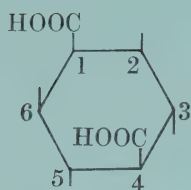
2,4,6/3,5-Pentahydroxycyclohexanone
(36)

* IUPAC Rule C-502 is compatible with a name 1L-6-*O*-methyl-1-thio-*chiro*-inositol for this compound, but that name does not accord with the instruction in Rule I-4.1 to use the "deoxy" nomenclature.





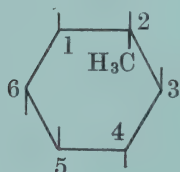
(1, 2, 4, 6/3, 5)-2, 3, 4, 5, 6-Pentahydroxycyclohexanecarboxylic acid (40)



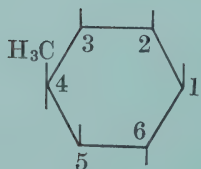
(1, 2, 4, 6/3, 5)-2, 3, 5, 6-Tetrahydroxy-1, 4-cyclohexanedicarboxylic acid (41)

I-4.3 Cyclitol derivatives in which one carbon atom carries a substituent additional to OH are named (i) as substituted cycloalkanepolyols or substituted inositols or (ii) as hydroxy derivatives, according as a substituent (i) does not or (ii) does rank above hydroxyl for citation as suffix. When the Rule leaves alternatives available, the criteria (ii) to (vi) of Rule I-3 are applied. For the disubstituted positions in such compounds the fractional prefix refers to the hydroxyl group and this may be specified for clarity where necessary.

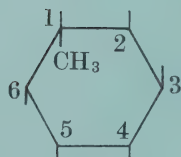
Examples:



2-*C*-Methyl-*myo*-inositol (42)

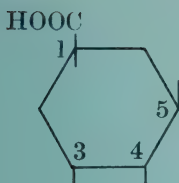


1D-4-*C*-Methyl-*myo*-inositol (43)*



1L-1-*C*-Methyl-*neo*-inositol (44)

* The prefix *C*- is added to denote substitution on carbon in accordance with carbohydrate nomenclature.

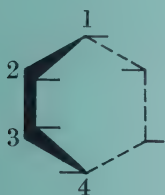


1L-1(OH), 3, 4/5-Tetrahydroxycyclohexane-carboxylic acid (45)
[preferred trivial name: (–)-quinic acid]

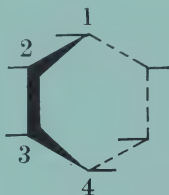
Note to Rule I-4: Replacement of the hydrogen of amino, mercapto, or hydroxy groups by other atoms or groups does not change the numbering of cyclitol derivatives except when it affects criterion (iv) or (v) of Rule I-3. However, the IUPAC Rules require that 'onium salts, acid, keto, nitrile, aldehyde, and derivatives thereof receive the locant 1; such cases will be relatively rare in cyclitol chemistry. A convenient alternative is to use the terminology exemplified by methiodide, hydrochloride, sulfate, etc.

Rule I-5 *Absolute configuration*

I-5.1 The absolute configuration is specified by making a vertical Fischer-Tollens type of projection of the structure, with C-1 at the top. The configuration is then designated as **D** if the hydroxyl group at the lowest-numbered chiral center (or other substituent if no hydroxyl group is present there) projects to the right, and as **L** if it projects to the left (cf. Figures I and II). This symbol, followed by a hyphen, is written before the name of the compound and may be preceded by the locant of the defining center. Racemic compounds are designated by a prefix **DL**.



I, **D**



II, **L**

Notes: (1) The mere absence of a prefix **D**, **L**, or **DL** indicates that the compound has a *meso*-configuration; thus, the prefix **D**, **L**, or **DL** should not be omitted.

(2) A simple way of applying this Rule is as follows: When the formula (drawn in the usual way, see Part A-3) is written with clockwise numbering and the substituent on the lowest-numbered asymmetric carbon atom is below the plane of the ring, the compound is **D**; if above, it is **L**.

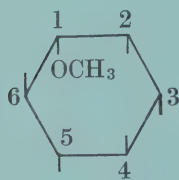
(3) In a great majority of cases the lowest-numbered chiral center is position 1, so that it would be reasonable that **D** or **L** should be preceded by the locant of the defining center only when it is *not* 1.

However, according to another nomenclature system for cyclitols¹⁰, and also for the related carbohydrate field, the symbols *D* and *L* are assigned to the *highest*-numbered chiral center, which sometimes gives symbols different from those assigned according to Rule I-5.1. It is, therefore, recommended that either the numeral 1 be included (as in these Rules) or a general statement be made in the paper concerned, for so long as confusion might arise.

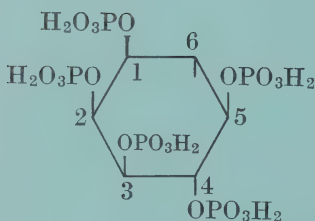
- (4) Small Roman capital letters should be used in print for *D* and *L*. For compounds containing cyclitol and protein or carbohydrate residues, *D_c* and *L_c* may be used alongside *D_s*, *L_s*, *D_g*, and *L_g* (cf. *J. Amer. Chem. Soc.*, 82, 5575-5576 (1960)).
- (5) When many OH groups are replaced by other substituents, it may be simpler to use the sequence rule⁴.

Examples:

Many examples of chiral compounds are named in the preceding Examples (e.g. 12-15, 17-20, 43). The following are additional.



1 *D*-1-*O*-Methyl-*myo*-inositol (46)



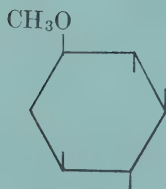
1 *D*-*myo*-Inositol 1, 2, 3, 4, 5-pentakis-(dihydrogen phosphate) (47)



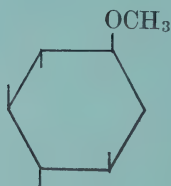
+



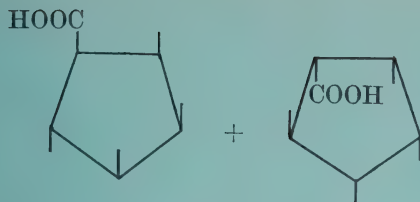
DL-*chiro*-Inositol (48)



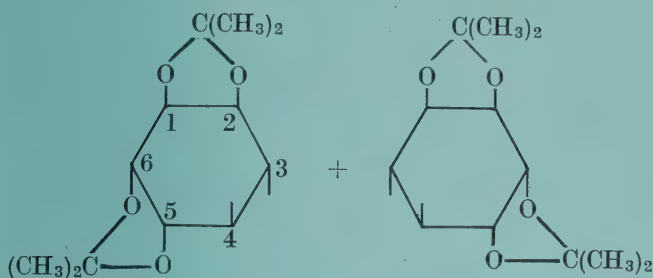
+



DL-1-*O*-Methyl-1, 3, 5/2, 4-cyclohexanepentol (49)



DL-(1, 2, 3, 4/5)-2, 3, 4, 5-Tetrahydroxycyclopentanecarboxylic acid (50)



DL-1, 2:5, 6-Di-*O*-isopropylidene-*chiro*-inositol (51)

See also Example (45), where the OH group and not the COOH determines the chirality prefix.

C. STANDARDIZED TRADITIONAL PROCEDURE

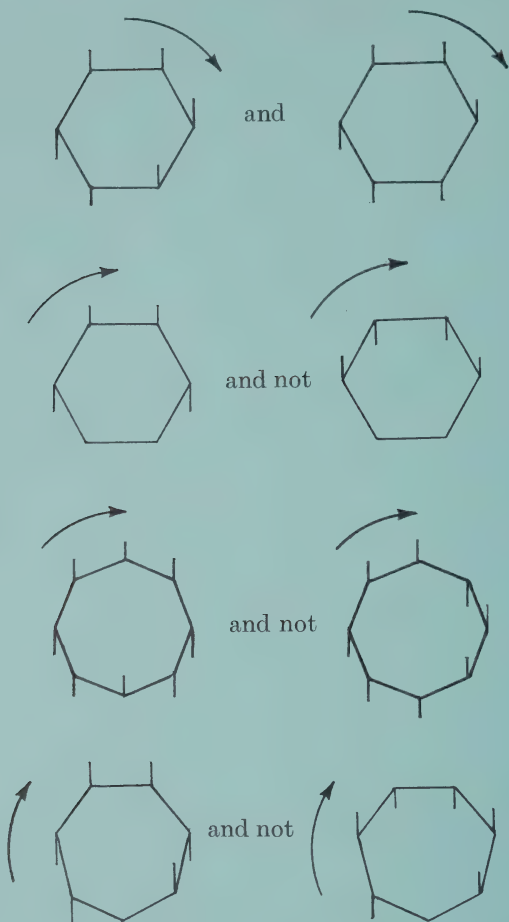
The significance of the Rules in this Part is discussed in the Introduction (Part A, p. 55). The numbers following the names in the Examples below are those that are arranged in numerical sequence in the Recommended Procedure (Part B); they are given for convenience of comparison.

The trivial names given in Rule I-1 of the Recommended Procedure (Part B) are accepted also for the Rules below, but the configurational prefixes are not italicized or followed by hyphens. The different numbering for dextrorotatory *chiro*inositol should be noted.

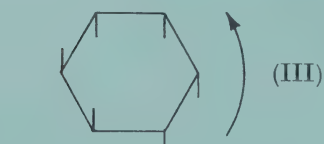
Rule A

Numbering is clockwise when the number of substituents above the plane of the ring is the same as, or greater than, the number below that plane. When alternatives remain, then (for clockwise numbering) the formula is orientated so that the substituents above the plane contain the greater number of adjacent *cis*-substituents and, if a choice still remains, the more compact set of *cis*-substituents.

Examples (arrows denote the direction of numbering):



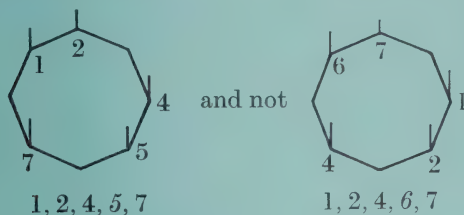
Note: This orientation of the formula is used below and is assumed in the numbering rules. Numbering is, however, anticlockwise if the formula is orientated in the opposite way, as in (III), so that the number of substituents above the plane is less than the number below it, but it simplifies interpretation if formulae are generally written as defined in the Rule.



Rule B

All the ring atoms of a cyclitol are numbered serially, the following criteria for lowest numbers being applied successively, so far as necessary to afford a decision: (a) all the substituents considered as one series; (b) substituents above the plane of the ring. The positional numbers (locants) are collected in front of the complete name of the compound, except that *O*-substituents precede the locants, with those for substituents above the plane (clockwise numbering) as numerator of a fraction and those for substituents below the plane as denominator, the locants in each set being in ascending numerical order; no further locants are required for the groups thus denoted.

Notes: (1) "Lowest" numbers are those that, when considered as a single ascending series, contain the lower number at the first point of difference, for instance:

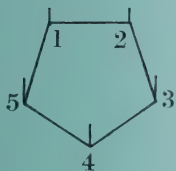


- 2) The fraction is written in these Rules on one line, e.g. 1, 2, 4/3, 5, 6-, but it may also be written, e.g. $\frac{1, 2, 4}{3, 5, 6}$ -.

Examples:

Effective
criterion

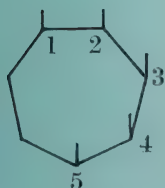
(a)



1, 2, 3, 4, 5/0-Cyclopentanepentol

(9)

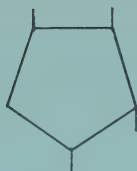
(a)



1, 2, 3, 4, 5/0-Cycloheptanepentol

(24)

(a)



1, 2/3, 4-Cyclopentanetetrol

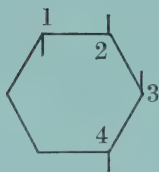
(a)



3, 4/1, 2-Cyclopentanetetrol

} Enantiomers (21)

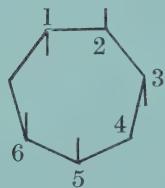
(a)



2, 3/1, 4-Cyclohexanetetrol

(22)

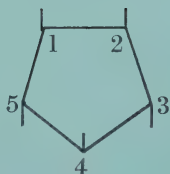
(a)



2, 5, 6/1, 3-Cycloheptanepentol

(25)

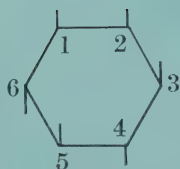
(a)



1, 2, 4/3, 5-Cyclopentanepentol

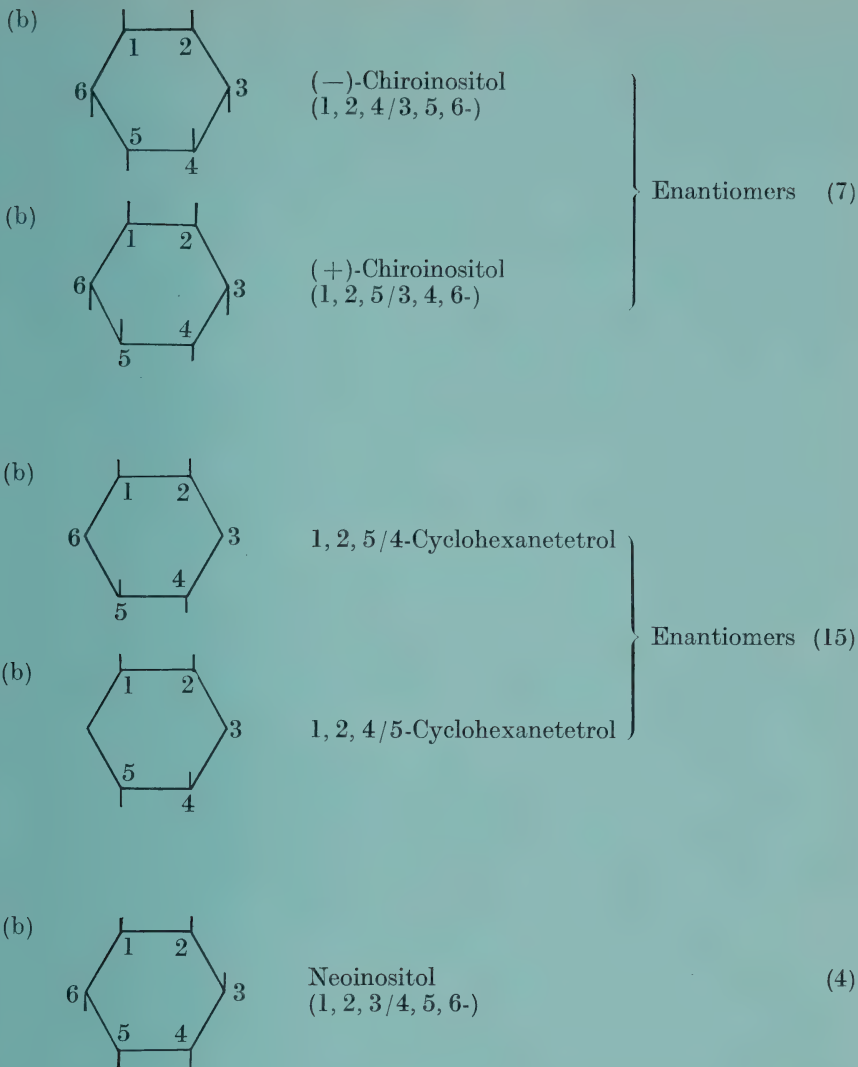
(26)

(b)



Myoinositol (1, 2, 3, 5/4, 6-)

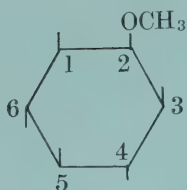
(5)



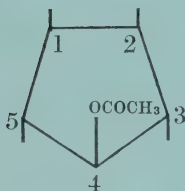
Rule C

When one or more hydroxyl groups of a cyclitol are (i) substituted by an alkyl, aryl, arylalkyl, or acyl group or (ii) replaced by an atom or group that according to the IUPAC 1965 Rules for the Nomenclature of Organic Chemistry, Section C, leaves OH with priority for citation as suffix, or when a cyclitol is substituted, the numbering of the parent cyclitol is retained; when alternative numberings are then possible, the standard rules of nomenclature are applied to decide between them so far as possible. The fractional prefix (if any) is placed after the names of *O*-substituents.

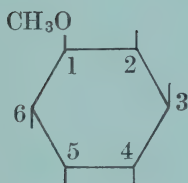
Examples:



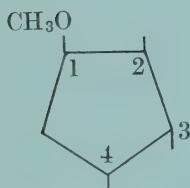
2-*O*-Methylmyoinositol (28)



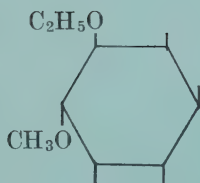
4-*O*-Acetyl-1,2,4/3,5-cyclopentanepentol (29)



1-*O*-Methylneoinositol (not 6-*O*-methyl) (18)

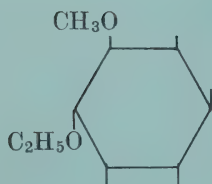


1-*O*-Methyl-1,2/3,4-cyclopentanetetrol (not 4-*O*-methyl) (19)

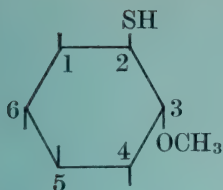


(a) Alphabetical order (*Chemical Abstracts*):
1-*O*-Ethyl-6-*O*-methylneoinositol (20 A)

or

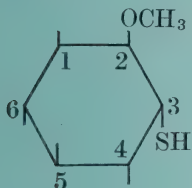


(b) Order of complexity (BEILSTEIN):
1-*O*-Methyl-6-*O*-ethylneoinositol (20 B)

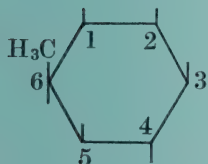


- (a) Alphabetical order (2, 2, 3 lower than 2, 3, 3):
2-Deoxy-2-mercapto-3-*O*-methyl-(+)-
chiroinositol (33A)

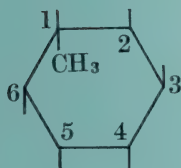
or



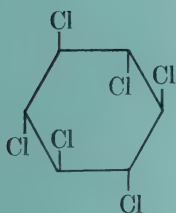
- (b) Order of complexity:
2-*O*-Methyl-3-mercapto-3-deoxy-(+)-
chiroinositol (33B)



- 6-*C*-Methylmyoinositol (43)



- 1-*C*-Methylneoinositol (44)

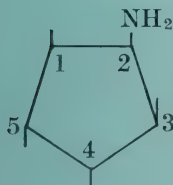


- 1, 3, 5/2, 4, 6-Hexachlorocyclohexane

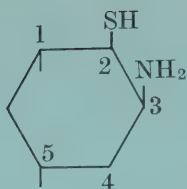
Rule D

When a hydroxyl group is replaced, the italicized symbol for the replacing group or atom may be added after the locant of this group or atom in the fractional symbol, no locant then being necessary in the alphabetical part of the name.

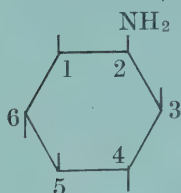
Examples:



- 1, 2*N*, 3/4, 5-Aminocyclopentanetetrol (34)



2*S*,3*N*/1,5-Aminomercaptocyclohexanediol (35)



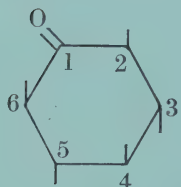
1,2*N*,3,5/4,6-Aminocyclohexanepentol (32)

Rule E

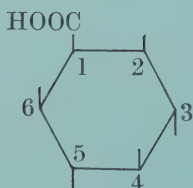
When a cyclitol derivative contains a group having priority over OH for citation as suffix according to the IUPAC 1965 Rules for Nomenclature of Organic Chemistry, Section C, then that group is numbered one, and this has priority over the criteria of Rule B.

Note: The groups in question are 'onium, acid, keto, nitrile, aldehyde, and derivatives thereof.

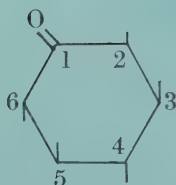
Examples:



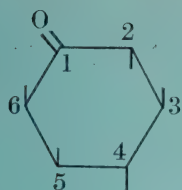
2,4,6/3,5-Pentahydroxycyclohexanone (36)



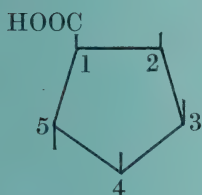
1(COOH), 2,4,6/3,5-Pentahydroxycyclohexanecarboxylic acid (40)



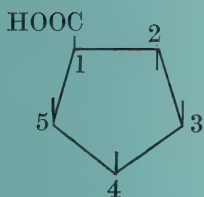
2,3,5/4,6-Pentahydroxycyclohexanone (37A)



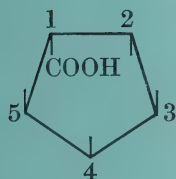
3, 5, 6/2, 4-Pentahydroxycyclohexanone (37B)
(Compounds 37A and 37B are enantiomers)



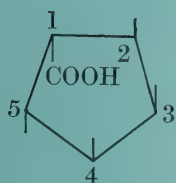
1(COOH), 2, 3, 4/5-Tetrahydroxycyclopentane-carboxylic acid (38A)



1(COOH), 3, 4, 5/2-Tetrahydroxycyclopentane-carboxylic acid (38B)
(Compounds 38A and 38B are enantiomers)



3, 4, 5/1(COOH), 2-Tetrahydroxycyclopentane-carboxylic acid (39A)



2, 3, 4/1(COOH), 5-Tetrahydroxycyclopentane-carboxylic acid (39B)
(Compounds 39A and 39B are enantiomers)

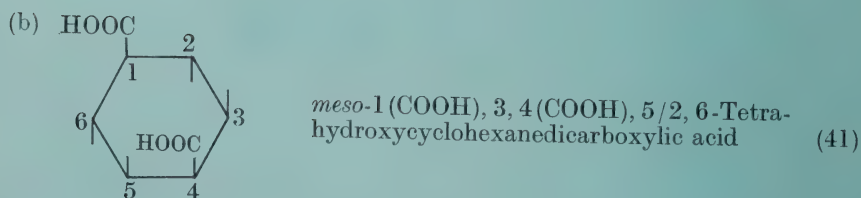
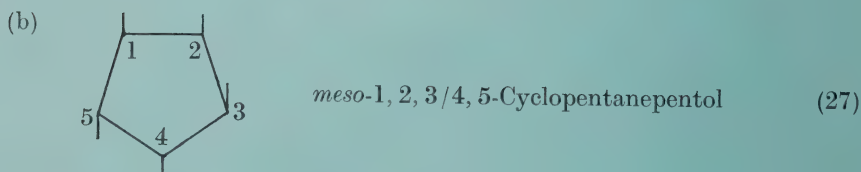
Rule F

(a) The rotation of an optically active cyclitol may be denoted by a prefix (+)- or (−)-* in front of the trivial name or positional fraction. (b) For a *meso*-compound the prefix *meso*- may be used. (c) For a racemic compound

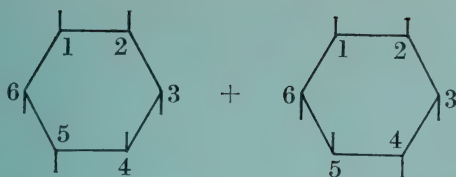
* Normally, (+)- or (−)- refers to sodium-D light, aqueous solution, and room temperature; if otherwise, the conditions should be noted.

the prefix (\pm)- or *rac.*- may be used, with the fractional notation that contains the lower numbers in the numerator, except that (d) for a racemic derivative of a compound with a *meso*-configuration each locant may be followed by its alternative in parentheses.

Examples:

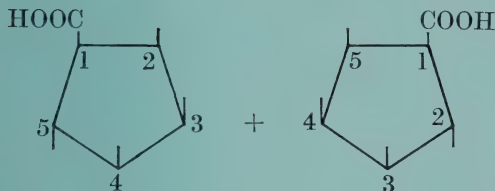


(c)



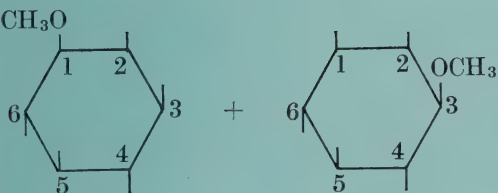
(\pm)-Chiroinositol
or (\pm)-1, 2, 4/3, 5, 6-Cyclohexanehexol (48)

(e)



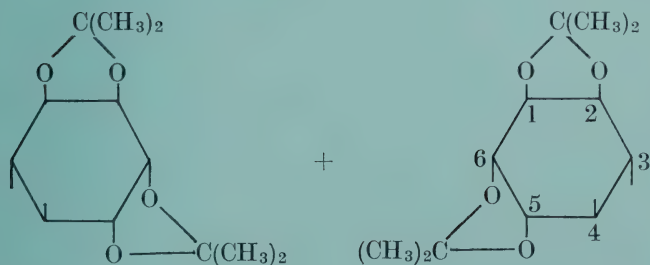
(\pm)-1(COOH), 2, 3, 4/5-Tetrahydroxycyclopentanecarboxylic acid (50)

(d)



1(3)-*O*-Methylmyoinositol
or (\pm)-1-*O*-Methylmyoinositol
or *rac*-1-*O*-Methylmyoinositol (cf. 46)

(c)



(\pm)-1, 2:5, 6-Di-*O*-isopropylidene-1, 2, 4/3, 5, 6-cyclohexanehexol (51)
or *rac*-1, 2:5, 6-Di-*O*-isopropylidene-1, 2, 4/3, 5, 6-cyclohexanehexol

References and Footnotes

- ¹Titular members: P.E. VERKADE (Chairman), L.C. CROSS, G.M. DYSON, G. KERSAINT, K.L. LOENING, N. LOZAC'H, H.S. NUTTING, S. VEIBEL. Associate members: R.S. CAHN, J. RIGAUDY. Observers: K.A. JENSEN, W. KLYNE.
- ²Members: O. HOFFMANN-OSTENHOF (Chairman), A.E. BRAUNSTEIN, W.E. COHN, J.S. FRUTON, P. KARLSON, B. KEIL, W. KLYNE, C. LIÉBECQ, E.C. SLATER, E.C. WEBB. Corresponding member: N. TAMIYA. Observer: S. VEIBEL.
- ³Members: S.J. ANGYAL (Chairman), L. ANDERSON, R.S. CAHN, R.M.C. DAWSON, O. HOFFMANN-OSTENHOF, W. KLYNE, TH. POSTERNAK.
- ⁴R.S. CAHN, Sir CRISTOPHER INGOLD, and V. PRELOG, *Angew.Chem.*, 78, 413 (1966); *Angew.Chem.internat.Edit.*, 5, 385 (1966).
- ⁵L. MAQUENNE: *Les sucres et leurs principaux dérivés*. Gauthiers-Villars, Paris 1900; also Georges Carré et C. Naud, Paris, 1900.
- ⁶TH. POSTERNAK: *The Cyclitols*. Hermann, Paris, 1965.
- ⁷IUPAC 1965 Rule C-16.4. *Pure and Applied Chem.*, II, Nos. 1-2 (1965).
- ⁸IUPAC 1965 Rule C-16.3. *Pure and Applied Chem.*, II, Nos. 1-2 (1965).
- ⁹K.R. HANSON, *J.Amer.Chem.Soc.*, 88, 2731 (1966).
- ¹⁰H.G. FLETCHER, Jr., L. ANDERSON, and H.A. LARDY, *J.Org.Chem.*, 16, 1238 (1951).

APPLIED CHEMISTRY DIVISION – PESTICIDES SECTION

Minutes of the second meeting of the Commission on Terminal Pesticide Residues

*held at 14.30 h on 27 August 1967 (and resumed at 14.30 h on
28 August 1967) in Vienna*

(1) Arising from the minutes of the first meeting, held on 25 November 1966, the chairman, Dr H. HURTIG, referred to the following matters:

(a) The recent publication of the report of the Joint Meeting of the FAO Working Party and the WHO Expert Committee on Pesticide Residues held in Geneva in November 1966 (FAO Report PL:CP/15) in which various problems concerning the nature of terminal residues, as summarized in Appendix I, were discussed. These problems were assigned by FAO/WHO to IUPAC and, through FAO/WHO, their solution would ultimately be of use to the FAO/WHO Codex Alimentarius Commission. Dr TURTLE and Dr WINTERINGHAM indicated arrangements which FAO (jointly with WHO) were making to receive toxicological information from industry.

(b) Further work on the nature of terminal residues of endosulfan, published in *J.Sci.Food Agric.* 18 (1967), 262–264 and *Residue Reviews* 21 (in press).

(c) A proposed symposium to be held jointly with IAEA, probably in October/November 1969, on “The Chemistry of Pesticide Metabolism and Terminal Residues”. The place would be decided after further consultation with FAO and WHO. Dr CÜTKOMP referred to various publications of IAEA which were of interest in connexion with possible methods of elucidating the nature of terminal residues (Appendix II); Dr WIDMARK referred also to possible uses of non-radioactive tracer work with mass spectrometry. The chairman stated that, when considering individual subjects, the Commission should bear four questions in mind: (a) what is the terminal residue problem; (b) who has posed it; (c) what IUPAC action, if any, should be taken in order to solve the problem; and (d) who is to progress any action required?

(2) The chairman referred to p.79 of the 1966 FAO/WHO Report (Appendix I) concerning *dichlorvos*, and Dr GALLEY introduced a discussion on the nature of terminal residues. Work on the metabolism in animals has been carried out by CASIDA and co-workers [*J.Agric.Food Chem.* 10 (1962), 208, 370] and the metabolic pathway elucidated. Rapid hydrolysis leads to dimethyl phosphate and methyl-2,2-dichlorodivinyl phosphate, further hydrolysis yielding monomethyl phosphate and inorganic phosphate together with dichloroacetaldehyde and dichloroethanol, the latter being excreted in the urine as a conjugate. Work was now in progress on the metabolism of *dichlorvos* by plants. Dr SUTHERLAND indicated that work was also in progress on potentiation studies for animal applications; work was also required on the nature of terminal residues in stored crops treated with *dichlorvos*. It was agreed that Dr GALLEY should coordinate information on the nature of terminal residues of *dichlorvos* (including information to be supplied by Dr PORTER and Dr RESNICK) for the Commission; and that this information would be passed to the chairman by the end of October 1967 for submission to the joint FAO/WHO meetings to be held in November 1967.

(3) The chairman referred to pp.131 and 141 of the 1966 FAO/WHO Report (Appendix I) concerning *gamma-BHC*; Dr VAN TIEL introduced a discussion on the nature of terminal residues arising from the use of *gamma-BHC* (Appendix III). Only a few publications dealt with the degradation products of *gamma-BHC* residues on food and plants; the mechanism of its degradation in houseflies has been studied, however, and the results had frequently been used as a guide to the food situation and many of the metabolites so found had in fact also been found in food. Future toxicological work might concern γ -2,3,4,5,6-pentachlorocyclohex-1-ene, 1,2,4-trichlorobenzene, m-dichlorobenzene and chlorobenzene and the apparent relative accumulation of beta-BHC in human fat and breast milk could be further considered. Dr WINTERINGHAM said that *gamma-BHC* was used extensively in rice in Japan. In further discussion it was also agreed that a more critical appraisal of the metabolic "balance sheet" in animal treatments appeared to be desirable and it was agreed that Dr HURTIG should explore the possibility of initiating work on terminal residues arising from the use of *gamma-BHC*, especially on plants and on rice in particular.

(4) Dr POLEN introduced a discussion as progress in the determination of the nature of terminal residues arising from the use of *chlordane*, these being virtually free of both heptachlor and heptachlor epoxide (Appendix IV). He described experimental work by Dr McCULLY, Dr KOIVISTOINEN, Dr WIDMARK and Dr WOODHAM which he was coordinating and which was now in progress, designed to evaluate (a) the effect of climatic conditions in terminal residue pattern and (b) the effect of cooking on terminal residues. It was agreed that Dr POLEN should continue to coordinate and progress the actions of his Working Group.

(5) The chairman referred to p.37 and p.45 of the 1966 FAO/WHO Report (Appendix I) concerning *carbaryl*; Dr SUTHERLAND introduced a discussion on the nature of the terminal residues arising from the use on plants of *carbamates*, including carbaryl, referring in particular to the evaluation which, together with Dr BARON, Dr BENSON, Mr COOK, Dr DOROUGH and Dr MOOREFIELD, he had prepared (Appendix V). Little of the mechanism proposed earlier for animals appeared to apply for plants, in which major hydroxylation occurred at the 4- and 5-positions with subsequent oxidation of the corresponding glycosides: there has also been a tentative proposal of a 5,6-diol. The benzene ring did not appear to be broken in any of these processes. He suggested that, so far as the identification of metabolites was concerned, the results obtained in stem-injection experiments should be confirmed by foliar application experiments. It was agreed that Dr SUTHERLAND should continue to coordinate and progress the action of his Working Group.

(6) Dr KORTE and Dr PORTER introduced a discussion on progress in the determination of the nature of terminal residues arising from the use of *cyclodiene compounds*. Dr PORTER said that a great deal of information on the metabolism of the cyclodiene insecticides in plants and animals had been published and that further studies were in progress. He outlined the general state of knowledge on this at the present time (Appendix VII). Whilst cyclodienes are usually very persistent when applied to the soil, they are biodegradable so that when there is free access to air they are less persistent. Almost all are converted to hydrophilic metabolites, but only major products have been identified; sunlight affects the chlorinated double bond. Chlordane gives two or possibly more metabolites. Heptachlor is converted to its epoxide and, as recently shown by KORTE, a metabolite. Aldrin is converted to dieldrin and each of these (together with endrin) in concentrated solution or in the solid state are transformed by internal H-capture; aldrin gives product and dieldrin product, the latter being highly toxic but meta-

bolized more rapidly than dieldrin. Other dieldrin metabolites have been identified in rat faeces and urine with further compounds in rabbit urine. The metabolites characterized so far in animals show little that is unusual but further work is in progress in a number of organizations. Less is known of metabolites in plants and soil but a number of people have indicated an intention to work on these. Dr KORTE said that endrin was very easily metabolized by rats, mosquito larvae, fungi and higher plants; heptachlor was quantitatively converted to its epoxide in animals and was readily excreted; but that isobenzan (telodrin) was to some extent stored by mammals and was excreted slowly as a hydrophilic metabolite (Appendix VI). Dr POLEN indicated that the conversion of heptachlor to hydroxy compounds was spontaneous and not biological in character. It was agreed that Dr PORTER should continue to coordinate information on the progress of knowledge of terminal residues of cyclodienes, particularly in plants, in collaboration with Dr KORTE.

(7) Dr SIJPESTEIJN referred to her publication with Dr VAN DER KERK in *Ann. Rev. Phytopath.* 3 (1965), 127, together with the publication "Metabolic Fate of Dithiocarbamates" by J. KASLANDER (Schotanus & Jens, Utrecht 1966), copies of both of which were circulated; and stated that little further information was yet available. Further work on bisdithiocarbamates and on the nature of the unknown dithiocarbamate degradation product in plants was intended. Dr RESNICK offered to enquire further about work on residues in man, and it was agreed that Dr HURTIG should consider means of making the need for further information on the breakdown products arising from the use of dithiocarbamates in plants more widely known.

(8) The chairman referred to pp. 108, 115 and 123 of the 1966 FAO/WHO Report (Appendix I) concerning ethylene dibromide and methyl bromide and Mr KENAGA introduced a discussion on the nature of the terminal residues of fumigants in general (Appendix VIII). He indicated the need to extend tracer studies for *methyl bromide* from wheat to other commodities such as cocoa and rice: Dr SUTHERLAND stressed the need to follow the fate of both halves of the molecule. In the meantime it would be useful, given analytical methods sensitive to 0.1 ppm, to conduct studies on the recovery of unchanged methyl bromide and of unchanged *ethylene dibromide* following fumigation: this indirect approach, whilst not the best, could give an interim indication of the extent to which products other than the original fumigants might be concerned. A reliable analytical method was needed to check amounts of unchanged *carbon disulphide* and work was necessary on the extent to which residues of *carbon tetrachloride* are removed by cooking: it was desirable that the latter should be supported by tracer degradation studies. Some new information was available on *ethylene dichloride* residues and Dr SUTHERLAND undertook to review this. There was little to report on chloropicrin, acrylonitrile (understood no longer to be used), ethylene oxide (some work on which including chlorohydrin formation was at present in progress) and propylene oxide. Mr COOK undertook to evaluate work on ethylene oxide. It was agreed that matters concerning methods for the determination of residues of unchanged methyl bromide and ethylene dibromide were referred to the Commission on Residue Analysis; and that Mr KENAGA should, with Mr COOK and Dr SUTHERLAND, coordinate information on the nature of the terminal residues of these and other fumigants.

(9) The chairman referred to pp. 214 and 226 of the 1966 FAO/WHO Report (Appendix I) concerning *rethrans* [*Chem. & Ind.* (1949), 636] and *synergists*. The secretary introduced a memorandum on the nature of terminal residues arising from the use of these on plants, which has been prepared by Dr THAIN and Mr FEUELL (Appendix IX) and Dr MOORE reviewed recent work, in-

cluding that at present in progress on metabolic pathways (Appendix X). Dr THAIN had indicated that it was more important to study residues of original rethrin than to study the nature and amount of terminal residues since when modified (by cleavage, polymerization, oxidation or reduction) the rethrin molecule showed a dramatic fall in biological activity. Dr MOORE indicated the occurrence of formates and carbon dioxide as metabolites of piperonyl butoxide but said that no study of the metabolic fate of MGK 264 was available. Studies on tropital were in progress and further studies on both this and piperonyl butoxide would commence shortly. It was recommended that Dr MOORE should, in collaboration with Dr THAIN, progress studies on the nature of terminal residues of rethrins and synergists (together where appropriate with studies of the extent of unchanged residues of rethrins either in the presence of synergists or otherwise), and coordinate information on these.

(10) Dr SUTHERLAND introduced a memorandum which, together with Dr SPENCER, he had prepared on the chemical nature of the terminal residues of *organophosphorus compounds* (Appendix XI). He stated that the situation was largely unchanged since the previous meeting of the Commission: there had been much work on a number of compounds but no new features had appeared. There appeared to be a dearth of information the metabolism by plants of *azinphos methyl* and (to some extent) *diazinon*: further work on *dimethoate* and *malathion* was in progress and such might also be required for *parathion* and *parathion methyl*. It was agreed to await further FAO comment on organophosphorus pesticides before referring the above matters to the Commission on Residue Analysis; and that in the meantime Dr SUTHERLAND should in collaboration with Dr SPENCER continue to coordinate information on the nature of the terminal residues of organophosphorus compounds with special reference to agricultural crops.

(11) The chairman announced that arrangements had been made to publish the proceedings of the meeting of the Commission held in November 1966 in the October issue of the *Journal of the Association of Official Analytical Chemists*. In this connexion it was agreed that 500 reprints of this publication, at an estimated cost of \$100, be purchased. It was agreed that whilst it was desirable that a summary of the proceedings of the present meeting also appear in this journal, much more original information had become available to the Commission; in view of this it was further agreed that IUPAC be requested to consider a full version of the Commissions proceedings (together with those of the Commission on Residue Analysis) should be prepared as a special IUPAC volume.

(12) It was agreed that the next meetings of the Commission should be held at Sittingbourne, Kent, England, in the period 12, 13, 14 June 1968 and that papers prepared for these should be in the hands of the Secretary by 15 April 1968. (*This arrangement was subsequently postponed*).

(13) At the joint meeting with the Pesticides Section which followed the meetings of the Commission, Dr HURTIG announced that the membership of the Commission had been agreed as follows:

Dr H. HURTIG (chairman), Dr H. EGAN (secretary), J. W. COOK, Dr R. A. E. GALLEY, Dr G. L. SUTHERLAND (members), E. E. KENAGA, Dr J. B. MOORE, Dr P. POLEN, Dr P. E. PORTER and Dr E. Y. SPENCER (associate members).

15 September 1967

H. EGAN

**Minutes of the second meeting of the
Commission on Development, Improvement and
Standardization of Methods of Pesticide Residue Analysis**

*held at 09.00 h on 28 August 1967 (and resumed at 09.00 h on
29 August 1967) in Vienna*

(1) Arising from the minutes of the first meeting, held on 26 November 1966, the chairman, Dr R. A. E. GALLEY, referred to the following matters:

(a) The recent publication of the report of the Joint Meeting of the FAO Working Party and the WHO Expert Committee on Pesticide Residues, held in Geneva in November 1966 (FAO Report PL:CP/15) in which some problems concerning residue analysis, as summarized in Appendix I, were discussed. These problems were assigned by FAO/WHO; their solution would ultimately be of use to the FAO/WHO Codex Alimentarius Commission. He also indicated various recommended tolerances and temporary practical residue limits for specific pesticides (most of which were available for the first time) as summarized in Appendix XVI. The meeting noted the views on methods of residue analysis expressed on p.26 of the 1966 Joint FAO/WHO Report; and expressed general agreement with the view that levels in milk of aldrin and dieldrin of 0.003 ppm and of heptachlor epoxide of 0.002 ppm were at a near to the general limit of detection for these compounds and it was emphasized that such analyses called for the use of professional analysts specially trained in the discipline of pesticide residue analysis with particular experience of organochlorine residue work at low levels.

(b) Dr RESNICK reported progress in collaborative work on methods of analysis for residues of *diphenyl*, stating that this had been by both EEC and by the TNO Central Institute for Nutrition and Food Research. EEC had been concerned both with the detection of diphenyl and with its estimation by thinlayer chromatography; the Secretary reported that, following correspondence with Dr SCHULLER, he had received a copy of the *Journal Officiel des Communautés Européennes* of 11 July 1967 which gave full practical details for this method. At the request of SA Cooperative Citrus Exchanges Ltd, the California-Arizona Citrus Industry, and the Citrus Marketing Board of Israel, TNO had also tested a gas-liquid chromatographic method for residues of diphenyl and considered this to be reliable and accurate for routine determinations: details were given in TNO Report No. R 2410 dated May 1967.

(c) Mr ELGAR reported that arrangements were being made to study different detectors in the gas chromatographic measurement of *dichlorvos* residues: the performance of electron capture, thermionic and flamephotometric detectors would be compared.

(d) Dr CUTKOMP reported on the International Atomic Energy Agency symposium "on Nuclear Activation Techniques in the Life Sciences" which had been held in Amsterdam on 8-12 May 1967, together with a meeting on 13 May (at which the Commission had been represented by Prof. WIDMARK) to discuss the problems arising from the contamination of the environment with various mercury compounds. A recommendation had been made that international collaboration should be initiated to organize the collection and provision of samples of biological material containing mercury, especially from areas likely to be above the natural background, and that arrangements be made for the assay of the mercury content of such samples. The IAEA Seibersdorf laboratories would be prepared to assist in the analyses.

It had also been recommended that international agencies should initiate and promote laboratory and field experiments designed to clarify the situation regarding the various forms of combination of mercury and the equilibria between these in nature. The Commission welcomed the prospect of collaboration and agreed to inform FAO/IAEA that if it was the intention to arrange collaborative studies IUPAC would be pleased to assist in the arrangements of these.

(2) The secretary referred to the following items of correspondence:

(a) With Dr H. J. Vos, secretary to IUPAC Oil and Fat Section, concerning possible help which the Commission might offer the Section when including in its methods compilation methods for residue analysis. This would be further discussed by the Section at its meetings in Prague on 30 and 31 August, after which specific proposal would probably be made to the Commissions.

(b) With Mr A. V. HOLDEN (Scotland), concerning the analysis of wild-life samples under arrangements sponsored by OECD. This subject had been discussed at the earlier meeting of the IUPAC Pesticide Section which had agreed that Dr WIDMARK should attend the OECD meeting on "Pesticide Residues in Wildlife" to be held in September 1967 as IUPAC observer; and that; together with Dr D. C. ABBOTT who would also be attending the meeting. Dr WIDMARK would assess the specific nature of any analytical problems for which IUPAC might be able to offer help.

(3) Mr COOK introduced a discussion on methods for the analysis of *organochlorine pesticide* residues, referring in particular to the evaluation which, together with Dr ABBOTT, Mr BLINN, Mr ELGAR and Dr McCULLY, he had prepared (Appendix XII). It was important to ensure completeness of sample extraction, difficulties in connexion with which had been encountered with dried fruits (which should always first be macerated with water) and with animal feeds. Thorough clean-up is essential if meaningful identifications are to be obtained: thin-layer chromatography is not the end-method of choice, but additional sensitive confirmatory tests are desirable. Dr SUTHERLAND agreed with these views and said that mass spectroscopy or infrared spectrometry were essential for the full confirmation of identity: nuclear magnetic resonance at present requires impracticably large samples. Dr TURTLE reinforced the need to confirm the identity of unknown residues and Dr EGAN referred to details set out in Minute 5 of the previous meeting of the Commission. It was agreed that four aspects in particular of organochlorine pesticide residue analysis warranted further work: the efficiency of sample extraction, the improvement of clean-up techniques, the specificity and selectivity of gas chromatographic detectors, and the development of further sensitive (and independent) confirmation techniques; and that Mr COOK should continue to collate progress in these individual fields and report this to the Commission.

(4) Dr FREHSE introduced a discussion on methods for the determination of residues of *organophosphorus pesticides*, considering the probable permissible levels for man for these in the light of information available in relation to the sensitivity of the analytical techniques at present in use and reviewing these techniques for the compounds *azinphos methyl*, *demeton*, *demeton-methyl sulphoxide*, *diazinon*, *dimethoate*, *fenitrothion*, *malathion*, *parathion*, *parathion-methyl* and *phosphamidon* (Appendix XIII). Both individual and multidetection methods of analysis are available for most of these; and whilst it is desirable that a more uniform multidetection procedure suitable for all (or most) of these were available, especially as regards the clean-up

procedure, with the possible exception of phosphamidon, the sensitivities of the methods appear to be adequate in relation to permissible levels and the possible tolerances derived therefrom. This conclusion assumes that the permissible level for fenitrothion is similar to that for parathion. These are only a few analytical methods dealing with specific metabolites, however, and there is a need to define the metabolites of toxicological significance before an evaluation of the methods available for their detection can be assessed. Dr McCULLY referred to work on the comparison of two gas chromatographic methods for organophosphorus pesticides at present being conducted by the AOAC, and Dr EGAN spoke of current work in the United Kingdom on the hydrolysis rates and products in foliar and cooking degradation studies. Dr HURTIG referred to the comments on multidetection systems of analysis contained in the Extract Report of the Second Meeting of the FAO Working Party on Pesticide Residues (FAO Report PL/1965/12, dated May 1966): this comment, which relates to multidetection systems in general, should be re-drafted in the light of present knowledge. It was agreed that Mr COOK, together with Dr ABBOTT, Dr FREHSE, Prof. KOIVISTONEN, Dr McCULLY, Dr SUTHERLAND and (if appropriate) Dr SPENCER should review this statement at an early date; and that on the assumption that a revised statement could be made available to FAO/WHO by November 1967, that Mr COOK together with Dr McCULLY should undertake any further revision of the statement which might become necessary in the light of later work, for the next meeting of the Commission. It was also agreed that Dr FREHSE should collate information on analytical methods for the degradation products of organophosphorus pesticides, especially where these were shown to be of toxicological significance, and to report progress in this matter.

(5) The chairman referred to p.199 of the 1966 FAO/WHO Report (Appendix I), concerning *organomercurial compounds* and to the report received earlier in the meeting from Dr CUTKOMP [Minute 1(d)]. Prof. WIDMARK added to Dr CUTKOMP's report and introduced a discussion on the residue analysis of these compounds (Appendix XIV), emphasizing that this was a specially difficult problem because of widespread distribution of traces of mercury in nature and (as recently discovered) the possibility of inorganically bound mercury being converted into alkylmercury in nature. Most of the analytical results available at the meeting in Amsterdam in May 1967 had been obtained by neutron activation analysis: other methods of adequate sensitivity were also available, such as atomic absorption spectroscopy, whilst mass spectroscopy appeared to be just at the limit of sensitivity required for the FAO/WHO practical residue limit of 0.02 to 0.05 ppm (Appendix XVI). He agreed that it was desirable that sensitive methods of analysis specifically for alkyl, alkoxy and aryl mercurials should be developed. It was desirable that radioactive methods should be compared with other methods, e.g. gas chromatography; however, aryl mercurials tend to decompose on gas chromatographic columns. Dr VAN TIEL reported work on water and wildlife in progress in the Netherlands. It was agreed that Prof. WIDMARK should continue to collate information on the progress development of methods of analysis for residues of specific organomercurials and to report this to the Commission.

(6) The chairman referred to pp.108 and 123 of the 1966 FAO/WHO Report (Appendix I) concerning methods of analysis for residue of unchanged *ethylene dibromide* and *methyl bromide* and referred to the recommendation earlier of the Commission on Terminal Residues for studies of the recovery of the fumigants from treated produce, provided that methods sensitive to 0.1 ppm were available (Minute 10 of the second meeting of the Commission on Terminal Residues). Members drew attention to the limitations of this approach in that relatively small residues of modified (and possibly more

toxic) compounds could not be detected with certainty, although it was understood that the Commission on Terminal Residues had regarded the recommendation as an interim measure pending further positive information on the nature of any other terminal residues derived from these fumigants. Dr TURTLE introduced a memorandum on methods for the analysis of residues arising from *ethylene dibromide*, *ethylene oxide*, *methyl bromide*, *phosphine* and various fumigant mixtures including *carbon disulphide* and *chlorinated hydrocarbons* which had been prepared by Mr BURNS BROWN (Appendix XV), referring particularly to work at Rehovot, Utrecht and Slough. Mr KENAGA referred to the Dow Chemical Company residue determination method No. ACR 62.12 for propargyl bromide residues in strawberries and cracked wheat. It was agreed that further work on the development of methods for residues of fumigants, particularly systems capable of detecting residues of several fumigants present together, was desirable and that Mr BURNS BROWN should be invited to collate information on the progress of this and to report to the Commission.

(7) The chairman referred to p.226 of the 1966 FAO/WHO Report (Appendix I) concerning rethrins [*Chem. & Ind.* (1949), 639], to the memorandum prepared by Dr THAIN and Mr FEUELL (Appendix IX) and to the recommendation earlier of the Commission on Terminal Residues that studies should be made on the extent to which unchanged residues of pyrethrins occur (Minute 11 of the meeting of the Commission on Terminal Residues). Dr MOORE reviewed methods for the determination of residues on food from sprays containing pyrethrins, piperonyl butoxide and MGK 264, including a biological method sensitive to 0.0035 ppm pyrethrins (Appendix X). Following discussion, it was agreed that it was desirable to develop clean-up methods for specific foods and that further work was also required on methods for the determination of synergist residues; and that Dr MOORE should continue, in collaboration as appropriate with Dr BRUCE, Mr LAUDANI, Dr PHILPERS and Dr THAIN, to report progress in these matters to the Commission.

(8) The chairman referred to arrangements for the publication of the proceedings of the Commission on Terminal Residues (Minute 13 of the meeting of that Commission); these arrangements were also agreed for the proceedings of the Commission on Residue Analysis.

(9) It was agreed that the next meetings of the Commission should be held at Sittingbourne, Kent, England, in the period 12, 13, 14 June 1968; and that papers prepared for these should be in the hands of the Secretary by 15 April 1968. (*This arrangement was subsequently postponed*).

(10) At the joint meeting with the Pesticides Section which followed the meetings of the Commission, Dr HURTIG announced that the membership of the Commission had been agreed as follows: Dr R. A. E. GALLEY (chairman), Dr H. EGAN (secretary), J. W. COOK, Dr H. FREHSE, Dr H. HURTIG, Dr C. RESNICK and Prof. G. WIDMARK (members), W. BURNS BROWN, K. E. ELGAR, Prof. P. E. KOIVISTOINEN and Dr K. A. McCULLY (associate members).

15 September 1967

H. EGAN

Appendix I

Further work indicated by the Joint Meeting of the FAO Working Party and the WHO Expert Committee on Pesticide Residues at the meeting held in Geneva in November 1966

Extracted from the report FAO PL:CP/15

Carbaryl (pp.37, 45) Several carbaryl metabolites have been identified in animals but not yet in plants. Excretion of carbaryl and its metabolites appears to be rapid in animals. Studies on the identification and toxicological evaluation of residues occurring in plants would be desirable. It is recommended that further work be done to establish more definitely the character of the terminal residue on treated plants.

Dichlorvos (p.79) Chemical nature of terminal residues occurring on foods from good pest control practices.

Dimethoate (p.232) Chemical composition and toxicity of the residues. Reproduction studies in the rat.

Diphenyl (p.93) A specification for diphenyl for use as a fungistatic agent on citrus seems desirable. The Working Party would like to receive further information on the likely impurities in commercial diphenyl.

Ethylene Dibromide (p.108) It should now be possible to develop a rapid, selective quantitative technique for traces of halogenated fumigants, together with suitable desorption techniques, and to combine these into a single method for the determination of residues in treated foods and the Working Party recommends accordingly.

Methyl Bromide (pp.115, 125) Chemical nature and amount of the residues in foods other than cereals. The Working Party considers that a sensitive multidetection method for residues of unchanged fumigants (including methyl bromide) in treated foods is now possible and the development of such a method would be a valuable advance.

gamma-BHC (pp.131, 141) The chemical nature of the residue occurring in plants has not been fully investigated. Data are needed on the disappearance of residues during storage and processing of food, and information on the chemical nature of terminal residues on food as consumed.

Organomercurials (p.199) Sensitive methods of analysis specifically for alkyl, alkoxy and aryl mercurials should be developed and used to study the occurrence of these forms of mercury in foodstuffs from different sources: these should include foodstuffs known to have been treated with specified compounds. Such analytical methods should also be used to study the possible conversion of aryl mercury compounds to more toxic ones.

Piperonyl Butoxide (p.214) Research should be conducted to determine the identity, persistency and toxicological effects of the breakdown products of piperonyl butoxide and the related compounds present with piperonyl butoxide.

Pyrethrin (p.226) Further work is needed on methods of detecting and measuring residues down to 0.1 ppm of pyrethrins. It would be useful to have the results of using such methods on a range of foods obtained in commerce.

Appendix II

Selected Bibliography of International Atomic Energy Agency Publications

Radioisotopes in the Detection of Pesticide Residues—(Panel Proceedings Series)

The report of a panel of experts convened in Vienna by the IAEA in April 1965. Various aspects of radiation and radioisotope applications to studies on pesticides were discussed and future lines of action were suggested. This publication contains the papers presented at the meeting together with the recommendations of the panel.

The Contents includes papers on the detection of residues in meat and milk, the metabolism of chlorinated insecticides, the chemical and physical nature of plant cuticles in relation to deposition and penetration of pesticides, neutron activation analysis of pesticides and metabolites, and other subjects.

Available in English only (116 pages, 16 × 24 cm, paper-bound, 25 figures; 1966). Price: US\$2.50.

Isotopes and Radiation in Plant Pathology—(Technical Reports Series, No. 66)

This report contains a collection of papers based on the papers originally presented at an IAEA panel of experts. Since the information is of direct use to plant pathologists, and since the subject matter is of great interest and covers a wide range, it was decided to make the revised papers available in published form.

The contents includes, amongst others, papers on the use of radioisotopes to study the spread of plant parasites, studies on the toxicity and mode of action of fungicides, the use of isotopes in plant virology, activation analysis in virus research, and the present status of the use of isotopes and radiation in plant pathology. Many bibliographical references are given.

Nine papers are in English and two are in French (94 pages, 16 × 24 cm, paper-bound; 1966). Price: US\$2.50.

Radiation and Radioisotopes applied to Insects of Agricultural Importance—(Proceedings Series)

Proceedings of a Symposium organized by the IAEA and the Food and Agriculture Organization and held in Athens, 22–26 April 1963. It had about 100 participants from 26 countries and five international organizations.

Contents: Insect ecology: tracer application (9 papers); Labelled insecticide studies: techniques (3 papers); Labelled insecticide studies: toxicology and residues (8 papers); Insect metabolism: tracer applications (3 papers); Radiation studies: principles and application of the sterile-male technique (4 papers); Radiation studies: specific effects (10 papers).

Each paper is in its original language with abstracts in English, French, Russian and Spanish. Discussions are in English. (508 pages, 16 × 24 cm, cloth-bound; 1963.) Price: US\$10.00.

Radioisotopes and Radiation in Entomology—(Proceedings Series)

Proceedings of an IAEA Symposium held at Bombay in December 1962. Papers by authors from nine countries deal with radioisotopes as tracers, radiation studies and insect problems in tropical countries. The Opening Address by H. J. BHABHA is also included.

Contents: Ecology and general biology (3 papers); Labelled insecticides studies (4 papers); Studies on insecticide resistance (2 papers); Insect physiology and biochemistry (4 papers); Studies on feeding behaviour (2 papers); Direct effects of radiation (4 papers); Using insects against themselves (3 papers); Some insect problems in tropical countries (3 papers).

Each paper is in its original language (21 English, 2 French and 1 Russian) and is preceded by an abstract in English, French, Russian and Spanish. Discussions are in English. (307 pages, 16 × 24 cm, cloth-bound, 79 figures; 1962.) Price: US\$6.50.

Radioisotopes in Tropical Medicine—(Proceedings Series)

Proceedings of a Symposium jointly organized by the IAEA and WHO at Bangkok in December 1960. The meeting was attended by participants from 20 countries and two international organizations.

The subjects include nutrition, protein metabolism and deficiencies, tropical sprue, haematological problems, iron metabolism, blood loss caused by parasites, haemolytic anaemia, endemic goitre, water and electrolytic balance, entomological problems, insect biochemistry, parasitology, helminth life cycles, protozoa.

Papers and discussions are in English, each paper being preceded by an abstract in English, French, Russian and Spanish. (375 pages, 16 × 24 cm, cloth-bound, 113 figures; 1962.) Price: US\$7.00.

(From: "Publications in the Nuclear Sciences, IAEA, 1967")

Appendix III

The Nature of Terminal Products arising from the Use of gamma-BHC

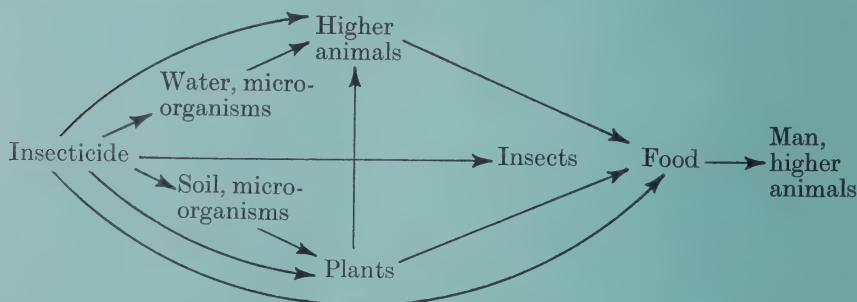
(1) Introduction

In considering the safety aspects of the use of gamma-BHC for agricultural, veterinary and various indoor applications, attention has hitherto been paid almost exclusively to the toxicological evaluation of gamma-BHC itself. As gamma-BHC, however, is known to be readily converted in biological systems, it is essential that further work be undertaken on the toxicology of compounds derived from gamma-BHC by biochemical degradation. Insufficient information on this point is available at present, and from existing literature data it seems that there is only little knowledge of the metabolism and degradation of gamma-BHC in plants and food, and of the nature of the terminal residues reaching the consumer [18]. The present report is an attempt to present as much as possible the literature data on these subjects in a concise form, so as to provide a basis on which the needs for further investigations can be more readily assessed.

As the chief aim of further work is to assess the toxicological properties of terminal residues of gamma-BHC, with a view of protecting the consumer, it is of prime importance to know more about the fate of gamma-BHC in food reaching the consumer, i.e. before as well as after processing.

Gamma-BHC can reach the food either directly, as the insecticide is currently being used for the control of pests in stored products, or indirectly by the treatment of plants or animals from which food products are derived. Consequently, the terminal residues reaching the consumer can be the result of degradation processes in the food itself or they can arrive in food products via such processes taking place in plants and/or animals. Through toxicological and biochemical work data are available on the fate of gamma-BHC in animals; however, such information is extremely scarce as far as plants are concerned. As it is known that gamma-BHC is being taken up by plants and animals after agricultural and veterinary application respectively, it is relevant to bear in mind any possible degradation process of gamma-BHC occurring prior to uptake, i.e. in the medium containing the insecticide. Such medium can be soil in case of soil treatment with gamma-BHC, or water in case of cattle or sheep dipping. In both instances it has been found that micro-organisms can cause a decomposition of gamma-BHC to other products which in turn could be taken up.

Much work has been done on the metabolism of gamma-BHC in insects, particularly houseflies. Although results of these investigations bear no direct relation with the present subject, they are included in the survey, as the data on metabolism in insects have been frequently used as a guide model for similar work in plants and food. For sake of convenience the survey on existing literature data is given under separate headings pertaining to the organism or medium in which the degradation process of gamma-BHC occurs. Figure I gives a diagrammatic illustration representing the routes via which gamma-BHC and its metabolites can reach the consumer, and the intermediate stages at which breakdown processes can occur.



(2) Food

BRIDGES [12, 13] has carried out an investigation on the retention of gamma-BHC after direct application to wheat and cheese, such as is practised in the control of pests in stored products, and on the fate of the insecticides during subsequent processing. Use was made of ^{14}C -labelled gamma-BHC, analyses being done by normal phase descending chromatography. Penetration of gamma-BHC in hard cheese (Cheddar) was found to be slow, residues equalling or exceeding the maximum permissible level (2.5 ppm) being only detected in the top 4–6 mm layer after 44 weeks of storage. There was, however, a greater penetration in soft cheese (Stilton), the tolerance being exceeded to a depth of 9 mm after the same period. Frequent applications of gamma-BHC to soft cheese were therefore considered inadvisable. The indications were that loss of gamma-BHC from cheese was generally slow, and in some parts of the treated material 40% of the initial dose remained for a period of 44 weeks after application. Gamma-BHC appeared to be unaf-

fectured by heating Cheddar cheese under conditions simulating the preparation of toasted cheese. No mention was made of other compounds being formed.

The experiments with wheat showed a rapid loss of gamma-BHC under conditions of aeration. Even at the highest dose of application (18.2 ppm) three weeks was sufficient for the residue level to fall below 2.5 ppm. However, complete loss was not attained even after prolonged aeration, suggesting that some of the insecticide is more firmly held in the lipoid content of the wheat. Wheat stored in closed containers did not show any substantial loss of insecticide even after 24 weeks. It was found that after the milling process the coarse bran contained about 2 to 4 times more gamma-BHC than the unmilled wheat, whereas the fine flour contained a residue of about 40 to 50 % of that in unmilled wheat. The use of bran for animal feed should therefore be regarded with much more reserve.

Further work on the fate of gamma-BHC residues in flour during the baking process revealed the presence of several breakdown products. It was shown that flour retained 30 to 40 % of the initial residue after heating and baking, the composition of the residue being as follows: gamma-BHC, 19.3 %; 1,2,3-trichlorobenzene, 6.3 %; 1,2,4-trichlorobenzene, 6.3 %; 1,3,5-trichlorobenzene, 2.3 %; dichlorobenzenes, 28.1 %; chlorobenzene, 7.6 %; and benzene (?), 1.0 %.

(3) *Plants*

The absorption of gamma-BHC in plants has been extensively studied by BRADBURY and WHITAKER [11], using ^{14}C -labelled insecticide. They found no indications that gamma-BHC was broken down to water-soluble products in wheat seedlings. The insecticide was lost by the plant probably due to volatilization of unchanged gamma-BHC, although the possibility of a volatile water-insoluble decomposition product was not *a priori* excluded. They quoted data from KOZLOVA and DVORTZOVA who reported that maize seedlings would be able to metabolize gamma-BHC. BOGDARINA [3] experimented with wheat seedlings grown in BHC-treated soil (isomer and purity of the insecticide was not indicated). It was presumed that part of the BHC was converted as a result of biological oxidation in which physiologically active plant constituents may be involved. The indication on which this assumption was based was an incomplete recovery (only 50 %) of BHC by absorption spectroscopy of aqueous extracts of seedling as opposed to complete recovery from seeds after swelling, and the lower toxicity to insects of young leaves as opposed to old leaves, which may be linked up with a more intense metabolism in young tissue.

More pertinent information on the metabolic fate of gamma-BHC in plants is given by the work of SAN ANTONIO [24], dealing with carrot, snap bean, tomato, potato, sweet potato, wheat and maize, grown in soil treated with gamma-BHC at various dosages. Extracts of the plant material were analysed by reversed phase paper chromatography, using *N,N*-dimethylformamide as immobile phase and *n*-hexane as mobile phase. The occurrence of one unknown metabolite of gamma-BHC was observed in carrots only, and the presence of this substance was ascertained in fibrous roots, edible roots, stem and leaves, the highest concentration being found in fibrous roots, which also contained the highest concentration of gamma-BHC. It was noted that the occurrence of the metabolite in carrots only was in accordance with the fact that this plant showed the highest accumulation of gamma-BHC as compared with the other plants examined. Analyses were also done of the soil adjacent to the roots, but no trace of the metabolite could be detected. As regards the nature of the metabolite, its possible identity with 1,2,4-trichlo-

robenzene or γ -2,3,4,5,6-pentachlorocyclohex-1-ene was further examined, as these substances have been found as metabolites of gamma-BHC in houseflies. On the grounds of its R_F -value the possibility of trichlorobenzene was ruled out, but the R_F -values of pentachlorocyclohexene and the metabolite were identical. Furthermore, both compounds gave rise to the formation of 1-chloro-2,4-dinitrobenzene after dechlorination and nitration.

It was concluded that the compound found in carrots as a metabolite of gamma-BHC may well be pentachlorocyclohexene or a closely related product.

(4) *Soil and micro-organisms*

BRADBURY [5] found evidence of loss of gamma-BHC in soil as a result of bacterial decomposition, but the indications were that the process proceeds slowly and is not completed eight months after application. Storage tests with different soils showed that loss is more rapid as the content of moisture and organic matter is higher. LICHTENSTEIN and SCHULZ [21] analysed samples of soil up to $3\frac{1}{2}$ years storage after treatment with gamma-BHC, both in laboratory and field experiments. Loss of insecticide was shown in all cases, but in addition it was found that the results of bioassay with *Drosophila melanogaster* gave not more than 60–70% of the recovery as found by chemical analysis in the 3-year storage tests, and only 46% in the $3\frac{1}{2}$ -year storage tests. This indicated the presence of a non-insecticidal metabolite which could not be shown by bioassay but reacted positively in chemical analysis. This was confirmed by YULE, CHIBA and MORLEY [18] who identified γ -2,3,4,5,6-pentachlorocyclohex-1-ene as a decomposition product in soil. This compound is approximately 1000 times less toxic to insects than gamma-BHC. Both micro-organisms and alkalinity of the soil are involved in the decomposition process [18].

(5) *Water and micro-organisms*

The effect of water and micro-organisms on the possible breakdown of gamma-BHC is only relevant in the context of veterinary applications such as cattle and sheep dipping, where the insecticide is in prolonged contact with the medium, and possible degradation products may be taken up by animals and subsequently lead to the presence of terminal residues of unknown toxicological properties.

From investigations by ALLAN [1] it is known that dipping liquid containing technical BHC (with 13% gamma-isomer) loses effectiveness which is not proportional to the loss of total isomers. It was found that this loss was due to bacterial decomposition of the gamma-isomer. The conditions of a cattle dipping bath were simulated in the laboratory by adding fine soil, cattle faeces and urine, and extracts from cattle hide scrapings at weekly intervals to a BHC suspension. Results of bioassay, using *Sitophilus granaria*, showed a greater loss after a few months than could be accounted for in the chemical analyses for total losses due to volatility were low. This indicated the formation of a non-insecticidal decomposition product. From experiments conducted with pure isomers it could be concluded that the gamma-isomer disappeared almost six times more rapidly than the alpha-isomer, the delta-isomer being intermediate, whereas there was hardly any loss of beta-isomer. Finally, it was shown that the growth of bacteria, such as *Clostridium sporogenes* and *Bacillus coli*, in a peptone serum bath containing gamma-BHC, was accompanied by a considerable degradation of the insecticide. It was postulated that hydrogen produced by the bacteria could possibly lead to dechlorination of BHC.

(6) *Insects*

Extensive work has been carried out by various investigators on the metabolism of gamma-BHC in insects, particularly houseflies (*Musca domestica*), mainly in connection with the resistance problem. Although this work bears no direct relevance to the object of this survey, it is considered useful to summarize the main results, because—as already mentioned above—the metabolic pathways of gamma-BHC in insects are often used as a guide model for similar work in plants and food. OPPENOORTH [22] in early work already established the breakdown of gamma-BHC particularly in resistant houseflies, and also found a similar degradation of alpha- and delta-isomer [23]. STERNBURG and KEARNS [25] found pentachlorocyclohexene as an intermediate in the metabolism of houseflies, and substantial quantities (up to 40% of the absorbed dose of gamma-BHC) could be detected particularly in the resistant strain. It was concluded that the compound is formed during the first few hours after treatment by topical application and that it may be consequently converted into other metabolites. Resistant flies produced pentachlorocyclohexene almost free from gamma-BHC 24 h after a 2–3-day residual exposure. BRADBURY [4], BRADBURY and STANDEN [6, 7, 9, 10] could not entirely confirm the above findings in houseflies. Experiments were carried out with ^{14}C -labelled pure isomers of BHC; analyses were done by paper chromatography, using vaseline as immobile phase and ethanol/water (10:1) as mobile phase.

Both carbontetrachloride and aqueous extracts were examined. Although initially no other compound than gamma-BHC could be found in the carbontetrachloride-soluble fraction, further examinations revealed the presence of a small amount of pentachlorocyclohexene (up to a maximum of 3% of the absorbed dose of gamma-BHC, an even smaller amount of 1,2,4-trichlorobenzene, and some unknown acidic compounds). Furthermore, some beta-BHC accumulated in the carbontetrachloride-soluble fraction to a larger extent than could be accounted for from the contamination of beta-isomer originally present in the radioactive gamma-BHC. All compounds other than gamma-BHC present in the carbontetrachloride-soluble fraction amounted to only 10% of the absorbed dose of gamma-BHC. The presence of only a very small amount of pentachlorocyclohexene was confirmed in subsequent work by BRIDGES [14], but ISIDIA and DAHM [20] failed to accumulate pentachlorocyclohexene in a reaction mixture of gamma-BHC and the breakdown enzyme, and concluded that it could only be a very transient metabolic product.

Analyses of the aqueous extract indicated the presence of a water-soluble metabolite. Quantitative experiments showed that all four common isomers are metabolized by both susceptible and resistant flies, but to a greater extent in resistant flies. Furthermore, alpha- and gamma-BHC are more readily converted than beta- and delta-BHC. In examining the aqueous extract by two-dimensional paper chromatography it was found that both alpha- and gamma-BHC produced eleven different compounds. Further experiments showed that alkaline hydrolysis produced dichlorothiophenols, all six isomers (2,3-, 2,4-, 2,5-, 2,6-, 3,4- and 3,5-) being present, with the 2,4-isomer predominating. These compounds totalled 68% of the water-soluble metabolites from alpha-BHC and 61% from gamma-BHC. *In-vitro* experiments showed that glutathione is a necessary co-factor for the enzyme responsible for the breakdown of BHC to water-soluble metabolites. This would infer that the metabolism involves the formation of a C-S bond. The nature of the original metabolites is unknown, but reference was made of a statement by WILLIAMS [26] that aryl mercapturic acids produced from halogen compounds by detoxification in mammals are also converted into

thiophenols by alkaline hydrolysis. Finally, it was found that a portion of the radioactive material was neither extractable by carbontetrachloride nor by water, and thus must be firmly bound chemically or by adsorption in the insect tissue.

Metabolism of gamma-BHC to water-soluble compounds has also been found in other insect species. This was shown by CLARK, MARGARET HITCHCOCK and SMITH [15] in cattle ticks (*Boophilus decoloratus*), who found S-(2,4-dichlorophenyl)glutathione to be the major metabolite; by BRADBURY and STANDEN [8] in malaria mosquitoes (*Anopheles gambiae*); and by BRADBURY [4] in khapra beetles (*Trogoderma granarium*), grain weevils (*Sitophilus granaria*), cockroaches and locusts. In general it was found that houseflies show an exceptional ability to metabolize BHC, as compared with other species, and it was postulated that this may well predispose this species to the development of resistance.

(7) Higher animals

No attempts will be made to give a full survey on all data regarding the toxicology of gamma-BHC and other isomers, or on the mammals. However, some existing information is presented here in as far as it is relevant to the present subject.

DAVIDOW and FRAWLEY [16] have carried out an investigation on the distribution, accumulation and elimination of the four common isomers of BHC in rats and dogs. It is known that in decreasing order, the sequence of acute oral toxicity is gamma-, alpha-, delta-, beta-; whereas on the other hand the order of chronic toxicity is beta-, alpha-, gamma-, delta-. It was shown that the degree of accumulation was correlated with the chronic toxicity of the various isomers. As regards distribution it was found that the BHC isomers were stored unchanged predominantly in the fat tissue, considerably lower amounts being present in brain, kidney, liver and muscle. No traces of 1,2,4-trichlorobenzene could be found. Elimination studies were carried out with weanling rats fed on a diet containing 100 ppm of the individual isomers for a period of 6 weeks. Analysis showed a rapid elimination of the alpha-, gamma- and delta-isomers (within 3 weeks), but the beta-isomer was persistent even after 14 weeks. On the other hand, VAN ASPEREN and OPPENOORTH [2] found no accumulation of gamma-BHC in mice after subcutaneous and intravenous injection. The insecticide was eliminated within 4 days and 1 day respectively, and the excreta contained no gamma-BHC or only negligible amounts. It was concluded that there is a rapid breakdown to unknown products. GROVER and SIMS [19] reported that 2,3,5- and 2,4,5-trichlorophenol could be found as metabolites in the urine of rats after injection with gamma-BHC, the latter compound being the predominant one. As both pentachlorocyclohexene and 1,2,4-trichlorobenzene yielded the same products it was assumed that these were intermediate metabolites. In addition another water-soluble metabolite was found in the urine, namely 2,4-dichlorophenylmercapturic acid, which was formed via a different metabolic pathway. It is interesting to note the similarities between rats and insects as regards the metabolic fate of gamma-BHC.

An interesting fact was revealed by work of EGAN *et al.* [17], who examined the presence of organo-chlorine pesticide residues in samples of human fat and human breast milk. As far as BHC is concerned all samples contained gamma-, beta- and gamma-BHC, but the beta-isomer predominated to the extent of 90% of total BHC in perirenal fat, whereas in breast milk nearly all BHC was present as beta-isomer. As beta-BHC is known to be the most toxic isomer chronically, these findings must certainly be considered of toxic

cological significance. The mean value of total BHC content amounted to 0.4 ppm in human fat, the content in human breast milk ranged from 0.009 to 0.033 ppm.

(8) Summary

The following is a brief summary of the nature of the metabolic products of gamma-BHC, some of which must be considered for future toxicological studies as they may be present as terminal residues reaching the consumer.

- | | |
|---------------------------------------|---|
| (a) Food (baked wheat flour) | 1,2,4-(and smaller amounts of 1,2,3- and 1,3,5-)trichlorobenzene
m-(and smaller amounts of o- and p-)dichlorobenzene
monochlorobenzene
benzene (?) |
| (b) Plants (wheat, maize)
(carrot) | unknown metabolite(s)
γ -2,3,4,5,6-pentachlorocyclohex-1-ene |
| (c) Soil and micro-organisms | γ -2,3,4,5,6-pentachlorocyclohex-1-ene |
| (d) Water and micro-organisms | unknown metabolite(s) |
| (e) Insects | γ -2,3,4,5,6-pentachlorocyclohex-1-ene
1,2,4-trichlorobenzene
unknown acidic carbontetrachloride-soluble metabolite(s)
11 different water-soluble metabolites giving 2,3-, 2,4-, 2,5-, 2,6-, 3,4- and 3,5-dichlorothiophenol on alkaline hydrolysis: possibly aryl mercapturic acid conjugates
unknown non-extractable metabolite(s) |
| (f) Higher animals | γ -2,3,4,5,6-pentachlorocyclohex-1-ene (intermediate)
1,2,4-trichlorobenzene (intermediate)
2,4,5-(and smaller amounts of 2,3,5-)trichlorophenol
2,4-dichlorophenyl mercapturic acid |

From the existing data it would seem that future work should be first directed towards elucidating the toxicological properties of γ -2,3,4,5,6-pentachlorocyclohex-1-ene, 1,2,4-trichlorobenzene, and in addition m-dichlorobenzene and monochlorobenzene. Furthermore, it is most desirable that work be undertaken to investigate the toxicological implications of the occurrence of beta-BHC in human fat and breast milk, as this compound seems to accumulate likely as a result of the large-scale use of technical BHC in many countries.

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N. VAN TIEL

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Appendix IV

Terminal Residues of Chlordane

The previous meeting of the Commission received evidence with respect to the constancy of composition of Technical Chlordane and the nature of its residues. The principle terminal residues were identified as alpha- and gamma-chlordane from characteristic "signature" gas-liquid chromatographic peaks. Neither heptachlor, a constituent of technical chlordane, nor heptachlor epoxide are manifested in the chromatograms of terminal residues. These compounds, if present at all, are construed to be a minute proportion of the terminal residues. The Commission agreed that a working group should be formed to further the knowledge about residues of chlordane. Elucidation of climatic and regional effects on weathering, fate of remaining residues in food processing, and systemic effects (where these exist) would comprise the mission.

A chlordane Working Party has been formed and experimental work is in progress. A status report has been submitted to the Secretary for conveyance to members of the Commission. The first project seeks basic information with respect to influences of weathering and cooking. The more complicated tasks of investigating systemic effects have been deferred until experience has been gained in management of an international scientific study. The present effort is directed toward securing qualitative information on chlordane treatment of two food crops which are cultivated in the diverse climates of (at least) North America and Europe. The investigation is designed as a time-ordered study of residue constituents on beans and cabbage. A study of the aging of chlordane residues has recently been reported by US FDA [13]. Reproductions of gas chromatograms demonstrate the progressive simplification of the residue pattern with time and the eventual dominance of two peaks which, whilst not named by the authors, appear to correspond to alpha- and gamma-chlordane. Fragmentary information indicates that

food processing is a probable means of removing residual chlordane from food. Experiments at the scales of pilot plant and commercial production of edible vegetable oils have demonstrated the complete removal of chlordane residues present in the crude vegetable oil. Process stages designated as deodorization and hydrogenation appeared to be particularly effective in producing the residue-free food products [7].

While it is recognized that our domain is elaboration on chemical and physical-chemical phenomena, these studies are strongly oriented by existing biological literature. To complement the bibliography on chlordane in the joint report of FAO/WHO (1965) [6], several additions are cited here. The items presented include studies on the toxicology of Technical Chlordane, fractions likely to contribute to residues, and pure isomers [1, 2, 3]; two new chronic feeding studies are introduced [4, 5]. Investigations have been made of the chemical, physical and biological interactions which take place when chlordane is applied to soil in agricultural situations [8, 9, 10, 11]. Rapid degradation of chlordane in soil has been observed and is attributed to microbial effects [11]. It has also been observed that chemical analysis generates higher apparent residue values than bioassay of the same soil; this discrepancy is attributed to the biological inactivation of chlordane by the soil [10]. There are also available a number of publications concerning studies on residues of chlordane in crops, finished foods, restaurant meals, etc. This literature is pertinent but does not form a sufficient basis for drawing conclusions about the specific problems before this Commission; therefore, it is not detailed here. Such data will, however, no doubt be of interest to FAO/WHO in their deliberations [12].

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Appendix V

Carbamates, including Carbaryl

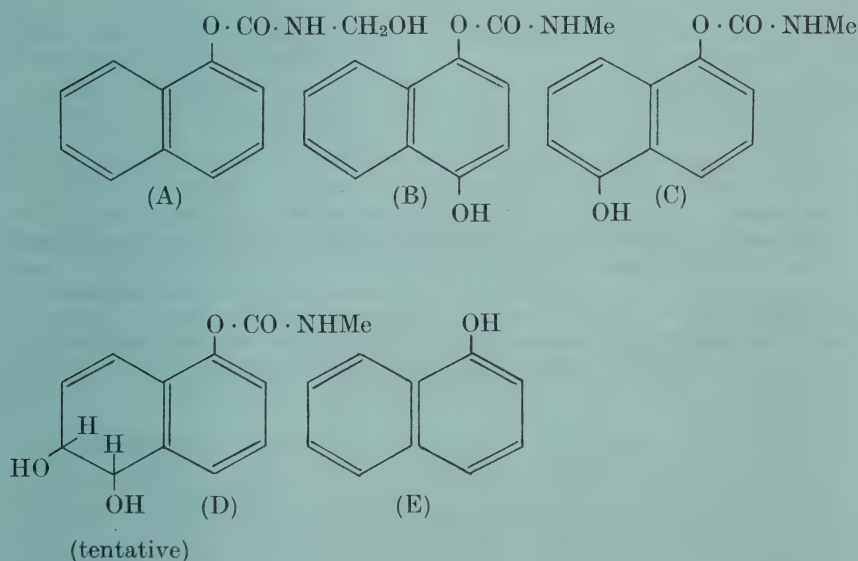
(1) Carbaryl

Since the November 1966 report to the Commission, several publications on the metabolism of carbaryl have become available or have been reported. Studies on the metabolism of the insecticide in mammals [1, 2] and insects [3, 4] have been reported and can be used to amplify earlier information. However, *in vitro* studies using animal (and plant) tissues [5] are considered to be of limited value for drawing conclusions on metabolism in intact animals. In plants the metabolic picture has not been as fully developed. A summation of the most recent material available pertinent to the entry and metabolic fate of carbaryl in plants follows.

The rate of dissipation of external pesticide residues from plants is determined by many independent factors. These include physical abrasion (wind), washing (rain) and volatility (heat, air, movement). In addition, chemicals changes occur on the surface due to oxidation (air), photo-oxidation (sunlight), and hydrolysis (humidity). The half-life of carbaryl on a glass surface was reported to be about one-third that found on the leaf surface, indicating a differential rate of dissipation dependent upon the texture of the surface. From 0.5 to 1 % of the initial dose underwent some chemical change prior to dissipation. Studies involving incorporation of carbaryl into plants suggests that root uptake is influenced by soil composition, water content, and microbial degradation [7]. Plants are more efficient in absorbing carbaryl through the root system than through the leaf surface. The bean plant removed 13 % of the carbaryl available from solution culture [8], cotton removed 40-47 % [9], and corn removed 63 % [10]. Measurements of the entrance of carbaryl into the plant resulting from foliar application indicated that this was not an efficient means of introduction. In corn, less than 2 % of the carbaryl applied locally to aerial portions penetrated the leaf surface [10]. Similar tests on the bean plant showed a foliar uptake of 2.6 % of the applied dose [8]. An early report demonstrating the passage of carbaryl into the rice plant [7, 11] showed that a more efficient movement of the pesticide occurred in the direction of roots to leaves rather than the reverse direction. Carbaryl may be considered to be a relatively immobile compound under conditions of foliar application. In cocoa, following root uptake, the maximum accumulation of carbaryl occurred in the apical regions of the leaves and in areas of active growth [12]. Since carbaryl does not readily penetrate plants when applied under normal agricultural procedures, abnormal conditions have been utilized to develop data on metabolism. Much of the data presented have been obtained when carbaryl has been artificially introduced in order to collect sufficient quantities of the by-products to facilitate experimentation and the characterization of metabolite.

Recent investigations in which ^{14}C -carbaryl labelled at three different sites (in the ring, the carbonyl carbon and the N-methyl group) was stem-injected into growing bean plants yielded the first insight into the fate of carbaryl in

plant tissues [13]. Serial harvests followed by homogenization, partitioning, etc., have shown that carbaryl is readily altered metabolically through both hydrolysis and hydroxylation. The 1-naphthol, the N-methylol carbaryl, the 4-hydroxy carbaryl, the 5-hydroxy carbaryl, and the 5,6-dihydro-5,6-dihydroxy carbaryl (tentative identification) metabolites are each conjugated with one of a series and are present in the plant as water-soluble beta-glycosides. The aglycones, liberated through *in-vitro* enzymatic action with β -glucosidase, are identical with the metabolites that have been identified previously from mammalian metabolism studies. The rate-limiting step in the plant appears to be the hydroxylation as the free aglycones were not detected in these experiments. Preliminary studies on bioassay of certain metabolites have indicated a reduced biological activity when compared with the present compound. Studies involving the liberated methylamine moiety in cotton suggest the formation of a water-soluble compound, minor evolution of a volatile basic substance (probably methylamine), and a small quantity of carbon dioxide [12]. By injecting carbaryl- ^{14}C labelled in the naphthyl ring, in the carbaryl carbon or in the N-methyl carbon into the stem of graining bean plants, aglycones (A) to (E) (see p. 101) have been identified after hydrolysis with beta-glucosides. The eventual plant metabolites are glycosides with mixed sugar moieties. These non-hydrolytic metabolites in many instances do not respond to the usual methods of analysis for carbaryl. This may be due to the fact that the metabolites yield a phenolic material different than 1-naphthol and do not show the same colour reaction or the solubilities are significantly different from carbaryl. These findings along with the lack of information on the toxicology of the metabolites impair the validity of the usual analytical procedures. Since a relatively small proportion of the applied chemical appears as radiolabelled metabolites, it is considered that no serious problem exists.



(2) Other carbamates

Recent reports of studies on the metabolism of other carbamates include: Temik ((*O*-methylcarbamoyl) oxime of 2-methyl, 2-(methylthio) propionaldehyde) in insects, plants [14] and mammals [15]; Banol (6-chloro-3,4-di-

methylphenyl methylcarbamate) in plants [16] and rats [17]; and NIA 10242 (2,3-dihydro-2,2-dimethyl-7-benzofuranyl methylcarbamate) in rats and bean plants [18]. The metabolism of the systematic insecticide Temik followed similar patterns in the insect and cotton plant [14], and mammal [15]. The sulfoxide analog was the principal nonhydrolytic metabolite. The persistence in plants of this active cholinesterase inhibitor was believed to be responsible for the long lasting systemic activity. Further oxidation of the sulfoxide to the sulfone along with the corresponding hydrolytic products was also observed. Metabolism of NIA 10242 by plants and mammals has been found to result in ring-oxidized carbamates and their corresponding conjugates [18]. Similar oxidation and conjugation has been reported with Banol in bean plants [16]. The principal metabolite was characterized as a phenyl glucoside containing the intact carbamate skeletal structure. A metabolite of Banol isolated from rat urine has been tentatively identified as an N-glucuronide of the intact carbamate [17]. A report of the photo-oxidation of two aminophenyl methyl-carbamates shows extensive degradation of the amino skeleton. This pattern of degradation would be expected to result in cholinesterase inhibitory metabolites on the surface of plants [19].

In general, studies on the metabolic fate of methylcarbamate esters as residues in and on plants and animals have resulted in elucidation of a pattern of oxidation followed by conjugation and either elimination (in the case of insects and mammals) or storage (in the case of plants). The toxicological significance of these oxidative and/or conjugated residues is unknown and should be considered for further investigations. The question of whether analytical procedures should be developed for the residues of unknown toxicological significance is of prime consideration.

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25 September 1967

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Appendix VI

Metabolism of Chlorinated Insecticides

An account of investigations carried out by Drs KLEIN, WEISGERBER, LUDWIG, PINONAWALLA and Messrs KATIL, MULLER, DHIRSAI and the author at the Radiochemical Laboratories of Bonn University.

On the occasion of the Panel on Radioisotopes in the Detection of Pesticide Residues, organized by the Joint FAO IAEA Division of Atomic Energy in Agriculture, Vienna, April 1965, results of investigations on metabolism of chlorinated insecticides were presented. These showed that aldrin, dieldrin, telodrin, chlordan, heptachlor and dihydroheptachlor are transformed to almost nontoxic hydrophilic products by mammals, mosquito larvae and fungi.

A fairly large number of metabolites were isolated and characterized by chromatography. Some of these could be shown to be identical, no matter whether the tests were carried out with fungi, larvae or mammals. The metabolites identified were hydroxy-derivatives of the insecticides administered. In long feeding trials with rats of both sexes with aldrin, a saturation level was reached after 50 days for males, 200 days for females. After intake ceased, the biological half-life period of residues for males is 11 days and for females 100 days. The metabolism takes place in liver, as indicated by bile-fistula experiments.

During the past two years we carried on these experiments on the metabolism of telodrin, heptachlor and dihydroheptachlor, with particular attention to the fate of endrin in mammals, insects, fungi and, for the first time, higher plants.

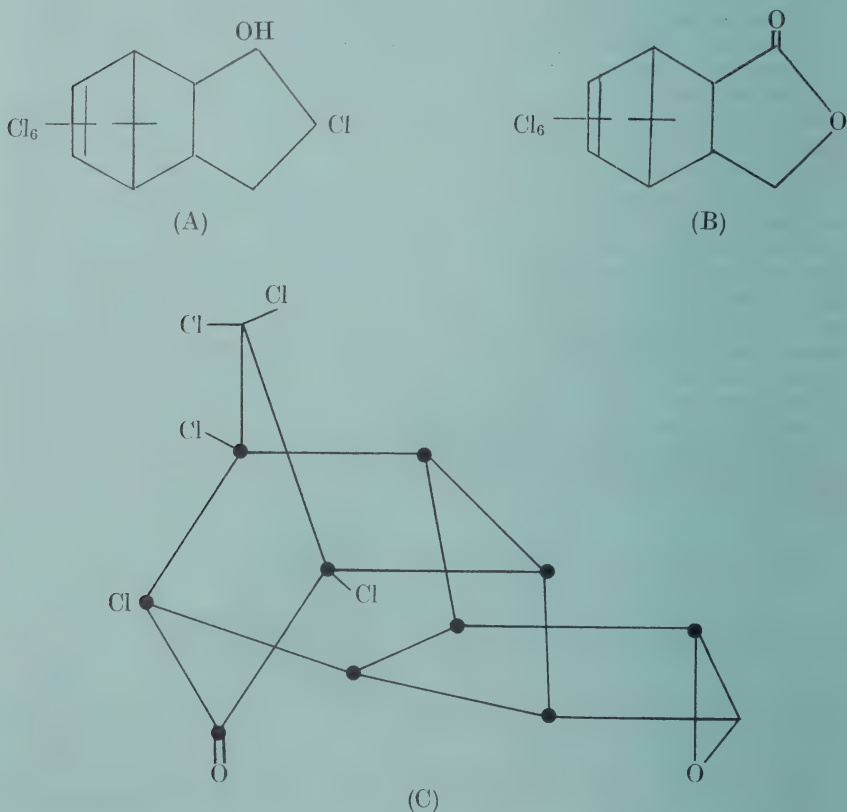
(1) Endrin

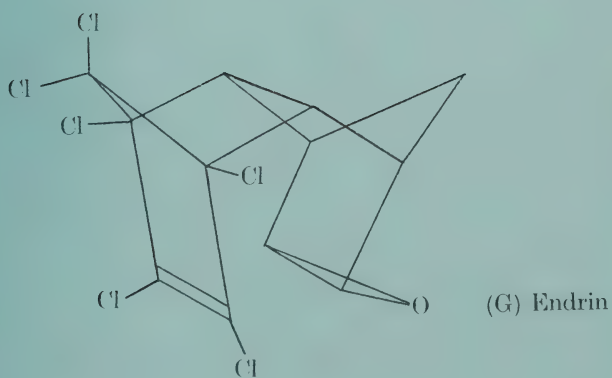
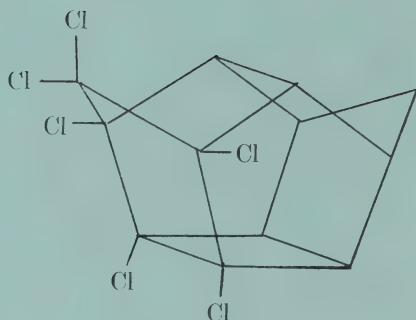
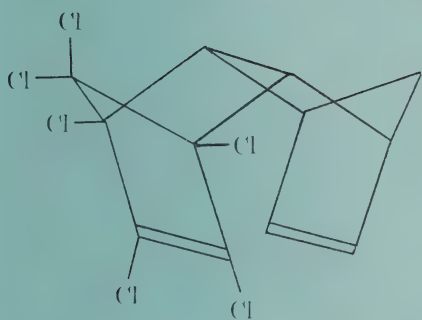
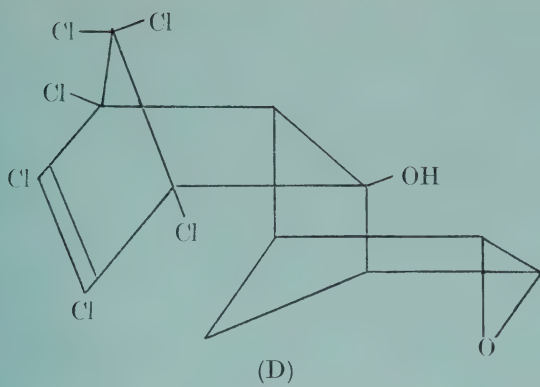
(a) Rats

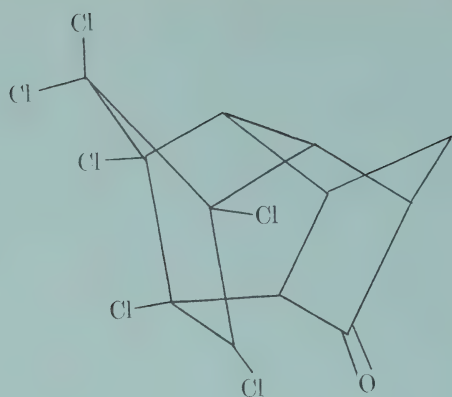
Wistar rats were used to determine the fate of endrin in mammals. Endrin-¹⁴C was applied both orally and intravenously. After oral administration in peanut-oil solution, endrin is quickly metabolized and excreted via the fecal route (less than 1% in urine). Excretion curves for various amounts of endrin applied to female rats (weight 250 g) are shown in Figure 1. These show that for the lower dosages half life of endrin is about two days and for the higher dosage of six days, indicating that the metabolic activity of rats is not proportional to the amount of activity applied: a greater proportion of the

128 $\mu\text{g/kg}$ dose being stored than for lower doses. In order to determine the steady state of storage and sex differences in the excretion rate, 3 male and 3 female rats (bodyweight 250 g) were given a daily dose of 8 μg endrin- ^{14}C for 12 days. As shown in Figure 2, 24 hours after the first dosage the male animals had excreted 60% of activity and the females 39%. After 5 to 6 days a steady state of storage was reached for all animals. 24 hours after the last application male rats had stored 14% of the total activity administered and the females 28%; after a further 3 days males still had 5.3% and females 15%. During the application of endrin- ^{14}C , the activity excreted consisted of 70 to 75% of hydrophilic metabolites. 24 hours after the last dose, endrin could no longer be detected in the excrements, the activity was then excreted only as metabolites. In another experiment 200 $\mu\text{g/kg}$ endrin- ^{14}C were injected in two portions into two rats of either sex, the excretion being measured of activity for 24 days. The exponential excretion curves are shown in Figure 3. In this case the biological half life of endrin was 2 to 3 days for males and 4 days for females. After intravenous administration no endrin could be detected in excrements. All of activity was excreted as metabolites.

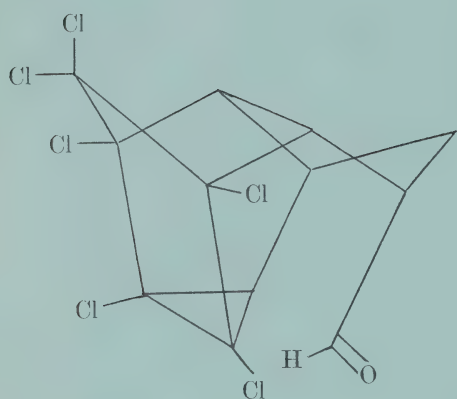
The metabolite fractions obtained from all experiments with rats consisted of one main metabolite, with only small amounts (less than 5%) of a second, still more hydrophilic one. The main metabolite is more hydrophilic than endrin and GLC-identical with the keto-rearrangement product of endrin (Figure 4) which occurs in technical endrin and is easily formed of endrin by heating or by UV-irradiation.



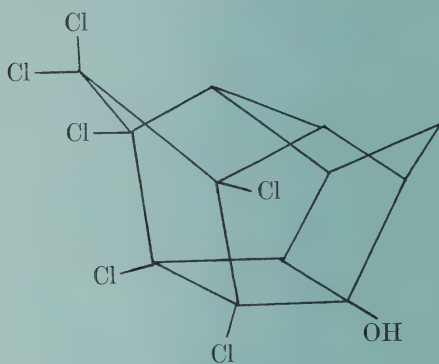




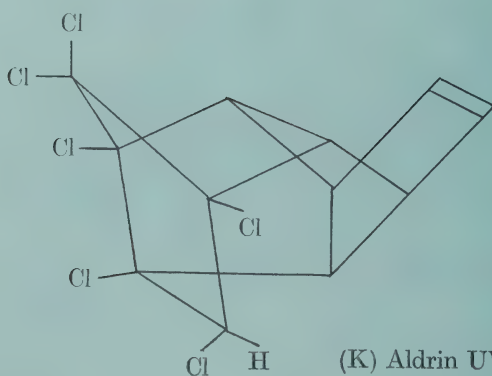
(H) Delta-keto-1,5,3



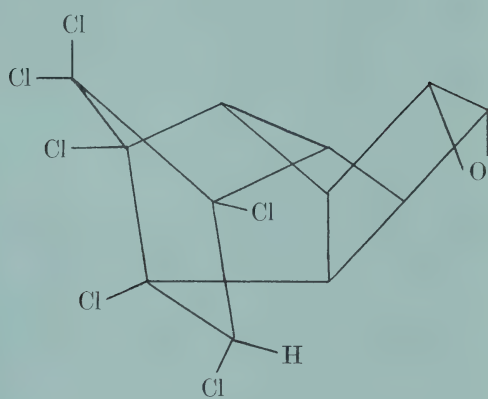
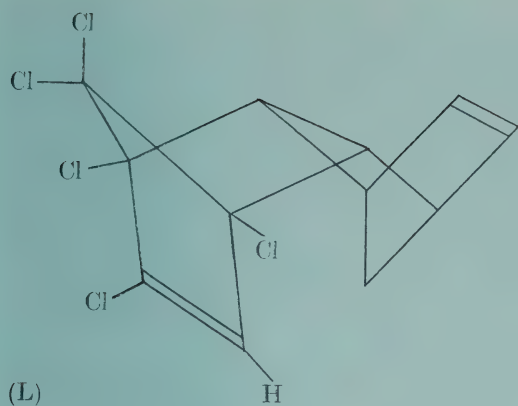
(I) SD 7442



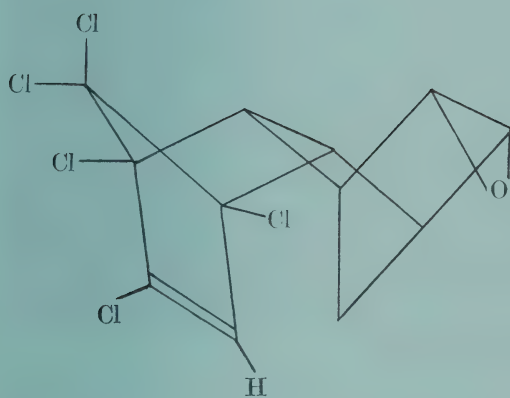
(J) "Bird cage" alcohol



(K) Aldrin UVCP



(M) Dieldrin UVCP



(N)

To determine the distribution of insecticide residues in the bodies, male rats were killed 24 hours after intravenous injection of 40 μg of endrin- ^{14}C (body weight 260 g). Table I shows the distribution of radioactivity in organs and tissues. A high amount of activity found in the tail is due to blood coagulation where the injection had been placed and is ignored since it did not enter the blood stream. This effect was only observed after injection of endrin and not with dieldrin, heptachlor or isobenzan (Telodrin). The distribution of activity after oral administration is given in Table II, which shows the change in distribution for the above animals one day after ceasing administration of endrin. The percentage, based on activity present in the bodies, increases in skin and subcutaneous fat, in abdominal fat and somewhat in the liver, but decreases rapidly—with exception of the liver—in the metabolizing organs, during these four days. Endrin itself is stored in the bodies: only traces of metabolites could be detected.

It had earlier been shown by bile-fistula experiments that the metabolism of dieldrin takes place in the liver. Homogenates of the liver did not change the insecticide. Endrin, too, is unchanged by homogenates of livers from cattle or pigs in Krebs-Ringer solution. The conversion of endrin is achieved after addition of NADH_2 to the homogenate solution. 100 g pig-liver in 300 ml Krebs-Ringer solution with 45 mg NADH_2 change 40% of 38 μg endrin to hydrophilic metabolites, which are identical with the products obtained by living organisms on incubation for 72 hours at 37 °C.

(b) Mosquito larvae

Up to now, only one note has been published on detoxication of endrin in insects. A component was detected in R- and S-houseflies which is chromatographically similar to the keto-compound. No excretion of metabolites could be detected [Brooks, G.T.: *Nature* (1960)]. In the present experiments larvae of a susceptible strain of *Aedes aegypti* were used. Since the amount of hydrophilic metabolites of dieldrin produced by *Aedes aegypti* depends on the consideration of insecticide in the nutrient solvent as well as on the amount of larvae used, we paid interest in these variations with endrin too. Since the metabolizing activity of larvae depends upon their age, we had also taken this in consideration. Endrin is changed by larvae of *Aedes aegypti* to hydrophilic substances which are to a great part excreted in the nutrient solution. We found up to 80% of the activity in solution due to metabolites and 50% metabolites in larvae. One-day old larvae have a very low metabolizing activity, only about 5% of applied insecticide being change within 24 hours. Small variations in insecticide concentration do not influence the rate of metabolism. When the insecticide concentration is increased tenfold in the nutrient solution, the rate of metabolism is only 10% higher. The metabolizing activity of larvae is greatest during the first hours of exposure, in one hour it may be up to 20% of the given dose. The distribution of activity between larvae and nutrient solution depends on the concentration of the insecticide and on the time of exposure; and is 20 to 70% in solution.

Only the living larvae metabolize endrin; homogenates in Krebs-Ringer solution as well as the nutrient solution itself caused no change of the insecticide. The extracted metabolites could be separated in three components by TLC, the concentrations ratio being 1:4:4. One of them has the chromatographic characteristics of the endrin-ketone.

(c) Plants

To define the fate of endrin in higher plants we used first cabbage (*Brassica oleracea* var. *capitata*). Young plants were used which had not yet formed

heads. Endrin- ^{14}C in acetone was dropped in various amounts on to the leaves. To avoid loss of activity by wetting only the soil was moistened in the greenhouse where the plants were cultivated. Two to four weeks after the application, leaves, stalks, roots and soil were separately worked up. The activity present on the surface was obtained by dipping the organs in methanol. The activity in the organs was extracted with methanol after homogenization. Only a small amount of the activity administered was found in plants and soil. This means that some of the insecticide applied evaporates before penetrating the plants. (Vapour pressure of endrin is 2×10^{-7} torr/25 °C.) By parallel experiments with silica gel plates and paper for chromatography the loss of activity on living plants was shown to be two times greater than found under these experimental conditions. The increase of the evaporation is probably caused by transpiration of the living plants. To design the slope of evaporated amount of radioactivity with time, several plants were treated with equal amounts of endrin- ^{14}C kept under constant conditions and worked up after intervals. The amount of endrin on the surface shows a declining slope and the amount in the plants itself too. After application of 50 μg endrin/plant, 66% of activity had evaporated within 2 weeks, 70% after 3 weeks, and 75% after 4 weeks. 10 to 25% of activity was recovered 4 weeks after application. Evaporation is greater under greenhouse conditions than when the plants are cultivated in small, badly ventilated boxes.

Most of the activity not evaporated was found in the plants as endrin and hydrophilic metabolites, whereas the small amounts on the surface were almost all due to endrin. Figure 5 shows the concentrations and rates of metabolism in the organs after administration of 500 μg endrin/plant. There is a concentration gradient from leaves and stalks to roots and soil for the total concentration of activity whereas the ratio of the metabolites to endrin increases from leaves to roots and soil. The water insoluble insecticide is probably stored mainly in the leaves after resorbance; the hydrophilic metabolites, on the contrary, are easily transported. Only 7% of the activity in the leaves is due to metabolites, 26% in stalks, 40% in roots and 51% in the soil, altogether 10.2% of the recovered activity. The metabolites found in soil were really excreted by the plants since degradation of endrin in soil itself is less than 5% within four weeks.

To decide whether the products are metabolites or artificial products formed by influence of light on active surfaces, some plants were kept in a darkroom for four weeks after endrin application. In these experiments the concentrations of metabolites in living organs were almost the same as in the plants which were kept in open light. Within the times used, endrin is degraded less than 1% by light or air since on the surface of the leaves only traces of metabolites could be detected: this was also true for faded leaves or on glass-plates and silica-gel plates kept in open light. The plant-metabolite fraction could be separated by TLC into two compounds, a very hydrophilic main-metabolite and a by-product which by GLC was found to be identical with the endrin-ketone. In another preliminary experiment with plants, young wheat germ buds were kept for 16 days on water containing 0.11 ppm endrin- ^{14}C . 58% of hydrophilic metabolites could be detected in the solution and 20% in the plants.

Fungi

Experiments to determinate metabolism of endrin by fungi were carried out with *Aspergillus flavus*. 0.13 ppm endrin- ^{14}C solution was first applied to growing cultures of the fungi. After three weeks cultivation, mycelia and nutrient solution were separately analyzed. Approximately 25% of radio-

activity was lost by evaporation and 3% of the applied dose were found in the cotton pads which were used to stopper the culture flasks (the pads contained only endrin, no metabolites, showing that no falsification of the measurements is caused by evaporation of metabolites). The distribution of activity under the experimental conditions used was almost independent on the concentrations of the insecticide. Figure 6 shows the distribution of endrin and metabolites in mycelia and culture media. Endrin was almost quantitatively resorbed by the mycelia and mainly stored. The metabolism rate is low and the metabolic products are quantitatively excreted into the nutrient solutions where 70 to 90% of activity could be detected as metabolites. The degradation rate of the total amount of activity present in mycelia and culture media is only 2 to 3%. An almost ten times greater metabolism rate was reached when endrin was applied (in 0.022 ppm concentration) to the culture media with fully grown mycelia. After three weeks of exposure the mycelia contained 20% of the activity as metabolites and the culture media 74% giving an overall metabolism rate of 22%. The metabolic fractions were separated by TLC into two components which by TLC and GLC are identical with the metabolites of cabbage.

(2) *Heptachlor*

Work on the storage, excretion and metabolism of heptachlor in mammals is described. When heptachlor is applied intravenously to rats or rabbits it is quantitatively transformed to metabolites. No trace of heptachlor itself could be detected in the excreta or in the bodies of the animals 72 hours after injection. After intravenous administration of 25 μ g heptachlor- 14 C to male and female rats giving an average concentration of 0.1 ppm in the bodies, the activity is mainly excreted in feces (as discussed for endrin). In Figure 7 the excretion, metabolism rate and sex differences are shown. Two metabolites (I and II) are present in various concentration ratios in the feces, whereas in urine only metabolite II could be detected. 72 hours after injection the rats were killed and the distribution of activity in the bodies was determined: results are shown in Figure 8. After administration to rabbits heptachlor is mainly excreted in urine and not in the feces (as earlier shown for other cyclodiene-insecticides). Within 144 hours after injection of 350 μ g heptachlor/kg body weight, male rabbits excrete 23% of activity as metabolites I and II (20% I, 80% II). Metabolite I (heptachlor *exo*-epoxide) was the main metabolite found in the bodies of rats and rabbits. Metabolite II could be detected also only indicating that this metabolite is quickly eliminated. Metabolite II is chromatographically identical (TLC, PC, GLC) with a synthetic sample of 1,2,3,4,8,8-hexachloro-5-*exo*hydroxy-6,7-*exo*epoxy-1,4,4a,7a,5,6-hexahydro-1,4-endomethylen-indene (IX) prepared and supplied by Dr G. Brooks, Slough.

(3) *beta-dihydroheptachlor*

In earlier experiments we had shown that beta-dihydroheptachlor is very quickly excreted as hydrophilic metabolites after intravenous administration to rats (75% within 72 hours). Preliminary investigations were carried out to see whether β -DHC is changed by microorganisms. After 15 days' exposure to *Aspergillus flavus*, *Penicillium urticae* and microorganisms from soil water to various concentrations of β -DHC, approximately 5% of breakdown products could be detected.

(4) *Isobenzan (Telodrin)*

Further experiments were carried out to determine the fate of isobenzan in mammals. Isobenzan- ^{14}C was administered intravenously in male and female rats. A hydrophilic metabolite was mainly excreted, with only traces of telodrin, in feces and urine. Males excreted with 48 hours 12% of administered activity in feces, 1% in urine; females 11% in feces and 5% in urine. The main amount of radioactivity excreted by rabbits is in urine, the rate of metabolism being 77%. Figure 10 shows the excretion of radioactivity by male rabbits. Isobenzan, with detectable amounts of metabolites, is stored in the bodies of the animals, mainly in fat, muscle and carcass. Figure 11 shows the distribution of radioactivity in organs and tissues of male and female rats after intravenous administration of $7\text{ }\mu\text{g}$ of isobenzan- ^{14}C /animal. The low amounts of isobenzan present in liver, heart and blood indicate that it is mainly stored and only slowly excreted. The natural metabolite of isobenzan has only recently been identified. After hydrolysis of the metabolite a substance is formed which is chromatographically identical to the known lactone (Figure 12).

July 1967

F. KORTE

Appendix VII

A Summary of Metabolism and Decomposition of Cyclodiene Insecticides in Plants and Animals

A great deal of information has accumulated in the literature regarding metabolism and decomposition of the cyclodiene insecticides in plants and animals. Further studies are now being made in a number of places, many stimulated by United States Government grants related to environmental contamination. Two recent reviews have appeared which discuss the available data [1, 2], so that no attempt will be made in this summary to completely catalog all of the experiments which have been done. Rather, an attempt will be made to present a general picture of the state of knowledge at the present time with a few extrapolations of the data into the realm of speculation.

(1) *Excretion and metabolism in animals*

In animals, evidence that the cyclodienes interact with metabolic processes was found very early. Aldrin, heptachlor, and isodrin were all found to be converted to their corresponding epoxides [3-6]. Further, when animals were fed, injected, or infused with various cyclodiene insecticides a number of general observations were made:

(a) When daily doses are given over a period of time, far more total insecticide can be administered without apparent toxic effects than would produce death when given as a single dose. This can generally be taken as an indication of a substantial rate of excretion or detoxification.

(b) With continuous administration of the insecticides in feed, the body content does not build up linearly with time, but reaches a saturation condition in which the rate of ingestion is balanced by the rate of elimination. This is particularly evident in the data of LUDWIG *et al.* [7] who continuously fed rats with ^{14}C -labelled aldrin and measured the excretion rates. Studies on ingestion of low levels of HEOD by humans over a period of fifteen months indicate that the saturation effect occurs also for humans [8]. Where analyses have been made of the excreta only small amounts of the parent compounds, or their epoxides in the case of aldrin and heptachlor, were found

in the urine or feces, the greater part being in the form of more polar metabolites. This will be discussed further in a later section.

(c) In continuous feeding studies after dosing is terminated or when a single dose is given, the body content of insecticide declines rather rapidly. In radiotracer experiments it is observed that elimination continues, and the rate of elimination declines logarithmically with time. It appears that in general the rate of elimination at any time is roughly proportional to body content [7, 9, 10].

(d) There is a simple relationship between the level at which an insecticide is continually fed to animals and the levels found in various tissues. Further, within a given species and sex, the ratio of stored pesticide in one tissue to that in another is fairly constant, even in the early unsteady state periods of feeding. Excretion in the milk of dairy cows is roughly proportional to the feeding level at any time and is fairly linearly related to content in body fat [11].

ROBINSON [12] has pointed out that these observations are compatible with a compartmental model such as is commonly used in the study of drug pharmacology. Such dynamic models have proved useful at least for smoothing data and for predicting equilibrium storage levels [9, 13]. One mathematical model which has closely fitted the data for a number of studies of cyclodiene insecticides in animals and which helps in intuitive reasoning is the very simple one described below. The analog of an animal can be taken to consist of two compartments, an active pool, and an average inert storage pool probably representing fat storage principally. It presumes that elimination rate is proportional to the amount of chemical in the active pool. Similarly, the rate of transfer from the active pool to the inactive pool is proportional to the amount in the active pool, and the reverse transfer is proportional to the amount in the inactive pool. Figure 1 diagrammatically shows these relationships with k_e , k , k_1 and k_2 , the respective rate constants. R represents the rate at which compound is introduced into the animal. It can be shown that if Q_A is the amount in the active pool, the solution for Q_A as a function of time t has the form:

$$Q_A/R = Ae^{-\alpha t} + Be^{-\beta t} + 1/k_e$$

in which A , B , α and β are all constants which are known functions of k_e , k_1 and k_2 . The solution for a feedoff period which $R = 0$ is simply:

$$Q_A/Q_A^0 = A'e^{-\alpha t} + B'e^{-\beta t}$$

in which the α and β are the same as before and A' and B' are very simply related to A and B .

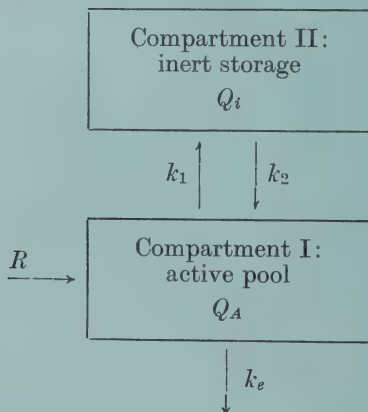


Fig. 1 Simple two-compartment model representation of an animal

It must be recognized in using such models that almost any curves can be fit with three adjustable parameters such as k_1 , k_2 and k_e ; however, the degree to which observed data for cyclodienes are represented is sufficiently good that the model above may be a very rough representation at least of what is actually going on. In many cases, and particularly for later stages in long feeding periods either the rate of change of Q_A becomes small, or the relative rates k_1 and k_2 are large with respect to k_e . Thus, at least as an approximation it can be assumed that Q_A and Q_i are in equilibrium or:

$$K = Q_i/Q_A = \frac{k_1}{k_2}$$

then:

$$Q_A = \frac{R}{k_e} (1 - e^{-k} e^t)$$

and the total quantity stored in the whole animal is:

$$Q = Q_A + Q_i = Q_A(1 + K)$$

$$Q = \frac{R}{k_e} (1 + K) (1 - e^{-k} e^t)$$

This approximate expression aids intuition in judging the possible effects of elimination rate constant and partition coefficient on total storage and rate of approach to steady state. The fit of observed data from feeding studies to the complete equation, and even to the simpler approximation provides some assurance that buildup of stored residues are in accord with expectations and reaches a maximum equilibrium value in relatively short times. POTTER [13] calculates that saturation times for aldrin and dieldrin in cattle are about 35–36 weeks; for endrin in cattle, about 6.9 weeks; for aldrin in male rats, about 7.5 weeks, and for aldrin in female rats, about 25 weeks.

A very significant study of the storage of dieldrin in humans has recently been reported by HUNTER [8]. 13 adult human males were used in a test of the effects of continuous deliberate ingestion of HEOD. 3 received 10 micrograms per day, 3 50 micrograms per day, and 3 211 micrograms per day. The remaining 4 received placebo doses as controls. During 15 months of test the concentrations of dieldrin in blood and adipose tissue were proportional to each other and to the rate of intake. The ratio of fat to blood concentration was about 156, and the ratio of fat content to intake rate was 0.67 ppm per microgram per kilogram per day. Storage results were in accordance with the simple model above with an exponential half life of about 25 weeks. Throughout the test none of the subjects complained of any symptoms and clinical observations remained normal and showed no significant trends. Upon the basis of the results and the average measured contents of the population of the United Kingdom, the average intake of HEOD is 25 micrograms per day per person, or about 0.33 micrograms per kilogram per day. It has been discovered that marked differences in storage of dieldrin and heptachlor epoxide are induced in animals by feeding DDT and some of its analogues [14–16]. The effect can also be produced by several enzyme-inducing drugs, and STREET has concluded that the DDT analogs have the effect of increasing the detoxifying enzyme activity in the animals. It appears that *in vivo* induction of detoxification may be useful for “cleaning out” contaminated animals. A great deal of interest has been focussed recently on non-specific hydroxylating, oxidizing enzyme systems requiring Reduced

Nicotinamide Adenine Dinucleotide Phosphate (NADPH) which are present in microsomal preparations, particularly from liver cells. These enzyme systems are commonly associated with drug metabolism and detoxification and are probably responsible for degradation of the cyclodiene insecticides *in vivo*.

WONG and TERRIERE [17] demonstrated *in vitro* that rat liver microsomal preparations with NADPH generating solution would rapidly epoxidize heptachlor, aldrin, and isodrin. There was no evidence, however, that the epoxides were further attacked. It was observed that sesamex inhibited the epoxidase action. Very significantly, the activities of microsomal preparations from male rats were much higher than those of females. Since it is commonly observed that female rats store dieldrin to a greater extent than males, the microsomal oxidation as a factor in k_e of the model discussed above seems likely. An elegant study by NAKATSUGAWA *et al.* [18] confirmed WONG and TERRIERE, and also determined that heptachlor, aldrin, and isodrin were converted to their epoxides, but not apparently further attacked under their conditions. Another significant finding which suggests a connection between the *in vitro* microsomal epoxidation, and *in vivo* detoxification, was the observation by GILLET *et al.* [19] that *in vitro* DDT analogs stimulate the microsomal epoxidize activity to aldrin and heptachlor in male rats and female quail. The induced enzyme seemed to have different properties from the normal enzyme. Some indications were obtained that dieldrin was slowly attacked by the enzyme system.

A number of workers have studied the metabolism of cyclodiene insecticides in insects [20-26]. The conversions of heptachlor, aldrin, and isodrin to their respective epoxides are well established. More investigators have not noticed further degradation, but KORTE *et al.* [26] showed that aldrin ^{14}C and dieldrin ^{14}C was further converted by mosquito larvae to at least four unidentified hydrophilic products. This conversion was confirmed in mosquitoes and shown to occur also in houseflies by GEROLT [25]. OONITHAN and MISKUS [24], using *Culex* mosquitoes, found a major hydrophilic metabolite of dieldrin, and showed that it corresponded in chromatographic properties to "aldrin glycol", 6,7-dihydroxy-6,7-dihydroaldrin. BOWMAN *et al.* [27] found that heptachlor and aldrin were converted to epoxides by mosquito larvae, but their extraction with hexane would not have detected more polar materials. They found 1-hydroxy chlordene to result from heptachlor treatments, but they found this to occur in the absence of mosquitoes as well.

In animals, the epoxidation of unchlorinated double bonds has already been discussed [3-6]. The further degradation of the epoxides to more hydrophilic materials is also well established and accounts for most of the detoxification and excretion. KUNZE and LAUG [28] fed rats with aldrin and dieldrin, and they noted that a toxic material to flies was present in the urine, liver, and kidney which was distinguishable from aldrin and dieldrin by its sensitivity to caustic. The material was present mainly in males, with only a small amount in females. CUETO and HAYES [29] reported finding metabolites of dieldrin in the urine from men exposed to dieldrin spray; however, they used an extraction with *n*-hexane which would probably not have recovered hydrophilic materials. HEATH and VANDEKAR [30], using ^{36}Cl -labelled dieldrin reported a metabolite of dieldrin in feces of rats which is more hydrophilic. They believed it to be a hydroxy compound which is excreted in the bile as a glucuronide. The urine also contained a similar material. More recently, DATTA *et al.* [31] studied urine and kidney tissue from rats fed with aldrin and dieldrin, using electron capture GLC as a detecting device. They extracted samples with ethyl ether and found two metabolites, the same for aldrin or dieldrin fed. One, with retention time three times aldrin on SF-96 stationary phase, was present in both males and females to about the same extent. The other metabolite at about 2.6 times aldrin was very

large in males, but only very small in females. Both disappeared on treatment with KOH. They found aldrin to be present in urine from dieldrin-treated animals, and it did not appear to be derived from impurities in the dieldrin administered to the animals. This might be worth exploring further, although the GLC peak is not a definitive identification of aldrin.

A great deal of information has been provided by KORTE, LUDWIG and their associates at the Bonn University [32-40]. They found that the cyclodiene insecticides are rapidly metabolized by rats and rabbits with the formation of materials which are much more hydrophilic. Extensive conversions of administered compounds were obtained in only 50 hours. In experiments with intravenous administration with a bile fistula it was determined that these conversions were the result of animal metabolism and not the action of microorganisms or fungi in the gut. Perfusion studies with rat livers using aldrin demonstrated conversion to dieldrin and more hydrophilic materials in the liver. In an experiment in which rats were fed aldrin in their diet over a long period of time, followed by a period on clean feed, LUDWIG *et al.* [7] found a big difference between male and female rats which could be accounted for by the much lower rate of metabolism in females. The compartmental model represents the data very well [13], showing the expected effects of the different k_e values on time constants and storage level. In early feeding stages the feces contained about 45 percent unchanged aldrin, 15 percent dieldrin, and 40 percent of hydrophilic materials and represented about 90 percent of total excretion. The urine at this time contained about 25 percent aldrin, 10 percent dieldrin, and 65 percent hydrophilic materials. After equilibrium was reached, the feces contained about 15 percent aldrin, 15 percent dieldrin, and 70 percent hydrophilic materials; the urine contained about 1 percent aldrin, 5-9 percent dieldrin and 90-94 percent hydrophilic materials. Chromatography indicated that the feces contained two hydrophilic components and the urine contained two. The main component in the feces was not the same as the main urine component, but the two by-products were apparently the same. Hydrolysis of the major urine component converted it to a new material with acid properties. This seems to agree with DATTA [31] and HEATH [30]. After feeding male and female rats with aldrin ^{14}C daily for three months, then sacrificing them, it was evident that metabolism of dieldrin was far slower in females than in males. The tissues of males contained large amounts of hydrophilic metabolites, comparable amounts of dieldrin, and little aldrin; female tissues contained very little hydrophilic metabolites or unchanged aldrin, but contained almost all of their radioactivity in the form of dieldrin. Dr KORTE has called attention to the possible relationship of these results to the results of *in vitro* microsomal oxidation.

The Bonn group have also examined hydrophilic metabolites of some cyclodienes in rabbits. Alpha-chlordane is almost entirely excreted in the form of hydrophilic metabolites, about $\frac{2}{3}$ in the urine and $\frac{1}{3}$ in feces. Two metabolites were present in the urine, partly conjugated. Metabolite A was found to be the chlorohydrine and based on comparisons with corresponding known alcohols, it was assigned the structure A. Metabolite B was more polar and was presumed to be the di-hydroxy compound resulting from displacement of the other chlorine. The acute oral toxicity of metabolite A was measured and it was found to be essentially non-toxic. No separations were apparently carried out on feces extracts to characterize their hydrophilic metabolites. In order to isolate metabolites of dieldrin, KORTE and ARENT [36] administered labelled dieldrin to rabbits twice a week for 21 weeks. Extracts of the urine with ether were separated on silica gel columns and then by thin-layer chromatography. Six metabolites were found of which one constituted 86 percent of the total and the other five ranged from

0.8 percent to 4.4 percent of the total. The predominant metabolite was purified and characterized as one of the optical isomers of trans-6,7-dihydroxy-dihydro-aldrin. It was optically active with a specific rotation of $(\alpha)_D^{20} = -13.7$. The same metabolite was also found in urine of rabbits which received intravenous administrations of aldrin [41]. Two of the other metabolites yielded the trans-diol on hydrolysis and are possibly mono- and diconjugated materials. The trans-diol metabolite was found to have a much lower toxicity than aldrin or dieldrin ($1/12$ to $1/18$ as great).

STIASNI [37] fed Telodrin insecticide to rats and isolated from the excreta the lactone B. This had also been isolated from treated mosquito larvae. Its acute oral toxicity to mammals was about 30-fold lower than that of Telodrin.

In toxicological studies at the Shell Tunstall Laboratories in England [42] it was found that extracts of both feces and urine gave gas chromatographic peaks which were not present in the excreta from rats fed a normal diet. Rats were fed six months on a diet containing 100 ppm of HEOD. They were then placed in metabolism cages and urine and feces were collected for one month. The urine was extracted with ether, the ether exchanged for hexane, and the extract was purified by liquid-liquid partition and thin-layer chromatography. About 0.5 milligram of metabolite was isolated. The feces were extracted with acetone, the acetone was evaporated to small volume, diluted with water, ferric chloride was added, and the sludge was extracted with hexane. The extract was purified by partition and by column and thin-layer chromatography to yield 12 milligrams of feces metabolite. The urine metabolite eluted from a gas chromatograph with a retention volume comparable to the major metabolite observed by DATTA [31] in male rat urine. Infrared spectrum indicated the presence of a carbonyl and an epoxide; it did not indicate a chlorinated double bond. The mass spectrum is characteristic of a molecule with five chlorines and the molecular weight based on ^{35}Cl is 358. The formula deduced is $\text{C}_{12}\text{H}_7\text{O}_2\text{Cl}_5$. The compound was said to form a dinitrophenyl hydrazone indicating the presence of a carbonyl. The suggested structure is indicated at C. The fecal metabolite differed from the urine metabolite. On GLC it was slightly less volatile. The infrared spectrum indicates a possible hindered OH group, tertiary OH group, a CH_2 , a chlorinated double bond, and an epoxide. NMR confirms a CH_2 group. The mass spectrum shows an ion of mass 359 with five chlorines, an ion of mass 347 with 6 chlorines, and an ion of mass 270 with 6 chlorines. It is proposed that the structure D is the probable metabolite. This is consistent with the findings of HEATH and VANDEKAR [30].

A recent study by CUETO and BIROS [68] has demonstrated traces of unconverted dieldrin in the urine from men and women from the general population. Levels ranging from 0.0005 to 0.0014 ppm were present in male urine, and 0.0011 to 0.0019 ppm in female urine. In men exposed to dieldrin occupationally 0.0053 ppm average was present with low exposure, 0.014 ppm with medium, and 0.051 ppm with high exposure. Identification was based upon retention times on three different GLC columns.

Endrin is inferred to be very rapidly metabolized because storage of endrin in the fat of animals is very low in comparison with other materials of similar partition coefficient [43-45]. LUDWIG [46] has measured excretion distribution and metabolism of endrin- ^{14}C by rats after intravenous administration. The endrin was administered to two rats of each sex at 2.1 mg per rat. After 48 hours the animals were sacrificed and excreta and tissues examined. About $\frac{1}{3}$ of the radioactivity remained in the tails where the injections had been made; it was unchanged endrin. Based upon the other $\frac{2}{3}$ the male rats eliminated 8.5 percent in the feces after 24 hours and 32 percent in feces after 48 hours; only 0.1 percent was in the urine after 48 hours. Corresponding

figures for females were 13.3 percent in feces at 24 hours, 24.5 percent in feces at 48 hours, and 0.3 percent in urine at 48 hours. The endrin remaining in both males and females was fairly uniformly distributed throughout the tissues. Analyses of extracts of feces yielded two different hydrophilic metabolites. No unchanged endrin was present and neither of the two metabolites was the common rearrangement product of endrin "delta-keto-153". The rate of endrin metabolism was much greater than observed for aldrin or dieldrin under similar conditions. LUDWIG [46] also administered endrin ^{14}C to a rat orally. The insecticide was administered daily in olive oil for eight days. Under these conditions endrin was eliminated at a very high rate. Steady state conditions were reached in only about three days, and after nine days, only 16 percent of the total administered dose remained in the body. 83.5 percent was excreted in the feces and only 0.5 percent in the urine. On the first day the feces contained 30% endrin and 70% metabolites; at steady state 25% endrin, 75% metabolites. Two metabolites were again found which appear to be the same as for intravenous infusion. Thorough studies of other cyclodiene compounds in animals do not seem to have been made.

(2) *Environmental degradation and metabolism in soil or plants*

The cyclodiene insecticides are less chemically reactive and more persistent generally than most other insecticides, and they have accordingly got an exaggerated reputation as environmental contaminants. In relation to organic chemicals, in general they are not particularly persistent and are vulnerable to degradation by physical, chemical, and biological actions. Under normal use conditions, ordinary reactions such as acid or base hydrolysis, oxidation, etc. would be extremely slow in all cases, and it is safe to assume that such mechanisms do not make major contributions to breakdown in the field. Light induced reactions and enzyme catalyzed reactions or metabolism by biological agents appear to be the principal sources of transformation.

In the late 1950's a number of workers noticed the sensitivity of cyclodiene compounds to ultraviolet light when making separations by thin-layer or paper chromatography. MITCHELL [47] published a study on the effects of ultraviolet light on a number of pesticides, which showed extensive conversions of cyclodiene compounds. Similar effects were noted by Shell laboratories at Birlinghoven, Germany, and Sittingbourne in England in connection with their work on metabolism of aldrin and dieldrin by mosquitoes and micro-organisms. Isodrin (E) was found to be converted by ultraviolet light into the "bird cage" structure (F) [48, 49]. This type of rearrangement is not uncommon in photo-chemistry when two double bonds are held sterically in such a favourable relationship. When endrin (G) is irradiated with ultraviolet light or with sunlight in solution or as solid, very rapid conversion takes place, principally to delta-keto-1,5,3 (H), with some SD 7442 (I), and minor amounts of other materials [50, 51]. Under alkaline conditions a further rearrangement of (I) to the "bird cage" alcohol (J) can occur. Confirmation of the structures of the above compounds has been based upon spectroscopic evidence and chemical reactivity and seems very solid.

In 1963 ROBURN [52] reported that photochemical conversion of dieldrin occurred on sprayed foliage. He noticed on a number of hay samples that a new peak was present in electron capture chromatograms of extracts from dieldrin-treated fields. He sprayed dieldrin on glass plates, irradiated the plates under a germicidal lamp for two to three hours, and found that the photo-product responsible for the new peak was formed in good yield. The work of ROBURN was confirmed by Shell laboratories in England and Ger-

many [53] and also by ROSEN at Rutgers University [51]. The studies of aldrin and dieldrin have been amplified by other workers [54-57], and a brief summary of the present situation is given below: When aldrin is irradiated with a germicidal lamp or mercury lamp in concentrated solutions or as solid in the absence of air, two main products are formed (K) and (L). In dilute solutions, CROSBY has found that (L) is predominant. When irradiation is done with ordinary sunlight, none of the isomer (L) is produced. CROSBY has shown that elimination of chlorine only occurs if radiation shorter than 2600 Å is used, whereas ordinary sunlight cuts off at about 2860 Å. In the presence of air, in addition to the above products, dieldrin is formed from aldrin, together with dieldrin transformation products. The irradiation of dieldrin in solution with mercury light leads to a tarry mixture of many products from which (M) and (N) can be isolated. If solid dieldrin is irradiated, very high yields of (M) are obtained while in dilute solutions (N) seems to predominate. As with aldrin, sunlight does not produce (N), since light of wavelength shorter than 2600 Å is required for the chlorine elimination. Sunlight rapidly produces isomer (M) which is stable.

SCHARF [58] explains the photochemical behaviour of aldrin, dieldrin, and endrin as deriving from the absorption of light to form an activated triplet state. This triplet state is likely to have the properties of an active diradical at the chlorinated double bond analogous to the well-known activation of a carbonyl group. In solution this radical can capture a hydrogen from the solvent leading to many possible products of free radical interaction, or it can lead to dissociation of Cl to produce (N). There are analogous reactions of alpha-halocarbonyl compounds. In compounds which have a hydrogen internally situated so that it is available to the diradical, the internal hydrogen can be captured leading to structures (J), (K), (M), and (N). No work has been reported on determination of the structures of photo-conversion products of other cyclodienes. They all suffer decomposition, but internal rearrangements are probably not likely with the principal insecticides heptachlor, chlordane, endosulfan, or telodrin.

The following table lists the acute oral toxicities of the compounds mentioned above which are of concern in connection with residues. The occurrence of residues on plants will be discussed in a later section.

Compound	Rats, LD ₅₀ , mg/kg
(F) "Bird cage" compound	>2000
(G) Endrin	25
(H) Delta-keto-1,5,3	62
(I) SD 7442	>2000
(J) "Bird cage alcohol"	250-400
(K) Aldrin UVCP	unknown
(L) Dieldrin UVCP	9.6

The Shell Tunstall laboratories have made some preliminary studies on the acute and subacute toxicities of the dieldrin photoisomer (L) [59]. They found (L) to be more acutely toxic than HEOD to rats, mice, guinea pigs, and pigeons. Domestic fowl and Harlequin fish were more sensitive to HEOD, while in Beagle hounds the toxicities of the two compounds were about equal. Chronic feeding of rats showed more rapid disappearance of (M) from the body than for HEOD. The biological half-life in depot fat for male rats was 1.7 days and for females 2.6 days. These values compare with 10 days and 13 days for dieldrin. This short half-life together with the observed low storage levels in the animals indicates that chronic toxicity of

the photoisomer should be very low. Under chronic feeding conditions the hazard from the dieldrin UVCP would be much lower than that of dieldrin itself.

The persistence of cyclodiene insecticides in the soil is extremely variable depending upon many factors such as temperature, degree of incorporation, moisture, organic matter, biological activity in the soil, and many others. EDWARDS [60] has reviewed the subject and lists the following times for 95 percent disappearance of the more common insecticides.

Chemical	Time for 95% disappearance, years	Average
Aldrin	1-6	3
Chlordane	3-5	4
DDT	4-30	10
Dieldrin	5-25	8
Heptachlor	3-5	3½
Lindane	3-10	6½
Telodrin	2-7	4

The stabilities are high and degradation is slow. A part of the losses from soil are caused by vaporization or co-distillation with water; it has been found by many workers that thorough incorporation into the soil and blanketing of the soil with a dense cover crop lead to longer persistence. There are large differences in persistence between sterile and non-sterile soil, and it is clear that a major source of degradation lies in breakdown by soil microorganisms. The products of this breakdown have not been studied except for the well-known conversions of aldrin to dieldrin and heptachlor to heptachlor epoxide. Further degradation products have not been found, but extraction procedures used would probably have missed water soluble products such as the diols and their conjugates. KORTE and his associates [26] shed some light on the breakdown by microorganisms in their studies with aldrin and dieldrin ¹⁴C. They found that cultures of *Aspergillus niger*, *Aspergillus flavus*, *Penicillium notatum*, and *Penicillium chrysogenum* converted aldrin into dieldrin and into four other components which may be two isomer pairs. The first of these pairs was water soluble. A culture isolated from compost-earth grew in a medium containing large amounts of aldrin forming the same products. Dieldrin was not converted by the organisms. CHACKO, LOCKWOOD, and FABIK [61] also found that dieldrin was not converted in culture by eight fungi or by nine different Actinomycetes. There is a great deal of interest in this area among University people as evidenced by request for radioactive samples for studies with microorganisms; however, little has so far been reported.

Large amounts of information on the residues of the parent compounds on crops are available, and will not be summarized here. Very little has been done on the metabolism of the cyclodienes in plants, but there is currently a great deal of activity which should clarify the picture in the near future. GLASSER [62] found a toxic compound in carrots grown in aldrin-treated soil, and this was later identified as dieldrin. LICHTENSTEIN and SCHULTZ [63] showed that aldrin and heptachlor are sorbed by roots of plants and converted to dieldrin and heptachlor epoxide. The epoxides are translocated in trace amounts into the foliage. Dieldrin and heptachlor epoxide are also sorbed and translocated, but no evidence of other products was found. Translocation of dieldrin and heptachlor epoxide have been demonstrated also by BRUCE *et al.* [64] and by SAHA and McDONALD [65] but levels in crops amount to only 0.01 to 0.02 ppm for high soil dosage rates. Studies of the extraction of root absorbed dieldrin from aerial parts of plants and of

the rate of translocation have been recently reported [66]. There is no indication of any metabolites. Very significantly no translocation of radioactive dieldrin could be detected when it was applied to plant surfaces. Absorption through the cuticle and translocation is negligible. A study has been made of the residues on cotton foliage resulting from endrin treatments [67]. Using tritiated endrin it was found that the total radioactivity dissipates rapidly. Endrin is the major constituent at all times with traces of "delta-keto-1,5,3" accounting for almost all the remainder. Presumably, conversion to delta-keto takes place, but this compound is lost more readily than endrin. Comparable results were reported by HARRISON *et al.* [54].

The most interesting metabolite residue of the cyclodiene compounds at present is the photoisomer of dieldrin (M). The other photoproduct (N) is not formed in sunlight and is of no concern as a residue. The high toxicity of the dieldrin UVCP has given rise to fears that high residues may occur in crop samples. The Shell laboratories at Woodstock have developed a highly specific residue procedure and have applied it to a variety of samples. The procedure is essentially the same as for dieldrin, with specificity afforded by the gas chromatography. Levels in crops grown in the USA seldom exceed 0.01 ppm and are usually below 0.001 ppm. Human fat samples from the USA were from a nationwide study conducted by HINE. It is significant that no residues of photoisomer occurred even when levels of dieldrin up to 0.25 to 0.3 ppm were present. As ROBURN had reported, very substantial residues of the photoisomer were present on range grass and wheat straw which had received foliar applications. One sample of apple pomace contained 0.06 ppm while dieldrin amounted to only 0.022 ppm; another apple sample contained about 0.03 ppm. The remainder of the samples had negligible traces or no photoisomer. HARRISON *et al.* [54] obtained similar residues for apples with both aldrin and dieldrin applications.

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Appendix VIII

Chemical Nature of the Terminal Residues of Fumigants Methyl Bromide

- (1) *How much unchanged methyl bromide is present in fumigated commodities, principally at the time of consumption?*

SHRADER and STENGER (1942) [2] report a method for methyl bromide sensitive to about 1 ppm which was used on flour and cheese. In this method methyl bromide is removed under conditions which lead to minimum decomposition and is determined by the difference between total bromide and inorganic bromide. By using this technique, methyl bromide was completely aerated from flour in 4 days. MAPES and SHRADER [3] also used a method which determines methyl bromide by difference between total bromide and inorganic bromide. It also can be used to analyze for ethylene dibromide. GERHARDT *et al.* [6] found that the total bromine residues in walnut meats treated with methyl bromide decline rapidly after fumigation and level off after 48 hours, indicating that most of the methyl bromide has volatilized. Since flour and walnut meats acquire rather high bromide residues compared to starches, sugars and certain fats, it is likely that flour and walnut meats also represent the more difficult aeration problems with methyl bromide. Thus, all but small amounts of methyl bromide, at the most, aerate rapidly from fumigated commodities before human consumption. The data do not offer unequivocal proof that all of the methyl bromide *per se* is or is not dissipated upon aeration.

Evidence that methyl bromide is not present in a fumigated commodity can be ascertained if no bromide (total of the organic and inorganic) residues occur or are present in no greater quantities than the untreated controls. A rapid method of such analysis of total bromide is that of X-ray fluorescence [4] although the sensitivity is only 5 ppm. By use of neutron activation methods (which requires no concentration steps) described by CASTRO and SCHMITT [5], detection of total bromide can be as little as 0.03 ppm. Even though the availability of the necessary equipment is limited to a few organi-

zations because of the expense and trained personnel involved, the method offers the best sensitivity for negative evidence of methyl bromide residues and can be used for experimental evidence. Positive evidence of methyl bromide in commodities might be possible by a modification of a gas chromatographic method for the determination of propargyl bromide [8]. The principle problem of modification for use with methyl bromide may be the capture of the fugitive gas for sampling purposes and possible background interference caused by the treated commodity. The background interference regulates the degree of sensitivity of the method which may be 0.1 ppm or less of the fumigant. BIELORAI and ALUMOT [10] describe an electron-capture gas chromatography method which allows detection of ppb of CCl_4 , CS_2 , chloroform and trichloroethylene. This method should be adaptable to methyl bromide.

- (2) *What are the methyl bromide reaction residues in fumigated commodities and their biological significance?*

Methyl bromide undergoes the typical reactions of an alkyl halide. Inorganic bromides are formed by hydrolysis and are naturally present in many unfumigated foods where they are well tolerated by man. Methanol, the other product of hydrolysis also occurs in small quantities. Typical reactivity includes methylation of OH, NH and SH bonds of amino acids and other proteins and SH groups of some enzymes [1]. Among the alkylated derivatives are N-methyl nicotinamide, methionine sulfonium methyl bromide, S-methyl l-methyl histidine. Some esterification of carboxyl esters are also thought to occur. It appears that such methylations do not block essential metabolism and often are readily reversible. LYNN [7] has well summarized the literature up to 1955. GETZENDANER *et al.* [9] have shown that certain food materials, such as cane sugar, macaroni, oleomargarine and butter pick up essentially no bromide residue following fumigation with methyl bromide, indicating no reaction with certain sugars, starches and fats, suggesting possibly that methylation is not readily accomplished in these commodities. These data also give support to the position that methyl bromide is rapidly and completely dissipated from fumigated commodities. Residues are modified by many physical and chemical factors related to the commodity such as exposure surface to volume ratio, solubility in the commodity, water content, etc. Temperature, length of exposure, degree of aeration, variable analytical techniques, etc., all make consistent correlation or bromide residues with given nutrient portions of food difficult to ascertain.

Conclusions

Providing an analytical method is developed with sensitivity to 0.01 to 0.1 ppm, it is suggested that a working party be formed to further elucidate the methyl bromide residues in a select list of commodities representing the major classes of foodstuffs.

Ethylene dibromide

Ethylene dibromide (EDB), which has properties of poor penetration into commodities and long retention, principally as the unchanged compound, was reviewed by the Joint Meeting of the FAO/WHO in March 1965 [1]. The inorganic residues considered to be of the same nature as those from methyl bromide and are treated as such. Grain containing $10 \times$ higher residues of EDB than normal, fed to chickens, caused a reduced egg size and produc-

tion [1]. AMIR and VOLCANI [12] found that EDB administered orally in high dosages in oil, as a capsule and in the diet, caused sperm abnormalities which disappeared after several weeks post-treatment. KAZMAIER and FULLER [13] found that confused flour beetle adults treated with sublethal dosages of EDB laid sterile eggs, while those treated with methyl bromide laid fertile eggs. This difference between methyl bromide and EDB may reflect their major physical and chemical properties, methyl bromide being more volatile, more easily hydrolyzed and retained only briefly as the unchanged fumigant in contrast to EDB. Thus, EDB fumigations have been known to interfere in the reproductive processes of mammals, birds and insects. EDB appears to remain unchanged for the most part in wheat. Ethylene glycol may be formed and reaction with methionine is possible [14]. Inorganic bromide is also formed, as with methyl bromide, by hydrolysis. It would appear that the major suspect for animal reproductive effects is EDB itself. The pertinent question which needs to be resolved is whether EDB leaves the grain completely upon a certain period of aeration (this may be highly variable and not dependable without analysis) or whether normal food processing and cooking will completely aerate EDB or hydrolyze it. The nature and the amount of bromide residue occurring as a result of fumigation with liquid grain fumigants containing EDB was determined by the use of radioactive bromine 82 [16], ethylene dibromide was completely adsorbed by wheat grain. About 50%, presumably EDB, was given off by heat treatment at 110–120 °C for 1 hour. The remaining bromide non-volatile compounds are only slightly extractable with organic solvents by Soxhlet extraction for 10 hours and are water soluble, probably a mixture of sodium and potassium bromide. After five days contact with the grain, 50% of the original EDB was changed to inorganic bromide. The remaining 50% can be volatilized in 59 hours in open air.

Contrary to the use of untreated grain for domestic animals and birds, man eats very little grain that is not processed in some way. EDB is lost from treated grain by turning, aeration, tempering, milling, etc., to a small percentage of the original level before cooking. STENGER and MAPES [17] showed that when wheat flour containing 8 ppm EDB was baked into bread rolls, the ethylene dibromide itself did not survive the baking process. The sensitivity of the analytical method used was 1 ppm of EDB. MUNSEY *et al.* [18] in a baking study, added 13 and 20 ppm of EDB ($10 \times$ the levels resulting from usual fumigations) to the flour and bread bases, prior to baking 1-pound loaves of bread. The analyses of the baked bread showed that there was no EDB *per se* remaining after baking within the limits of the sensitivity of the method, which was 1 ppm. Rolled oats treated to attain about $10 \times$ the expected residue level of EDB, quick cooked for one minute, reduced EDB 51% from 22.4 to 12 ppm. Considering normal processing procedure for producing rolled oats, it seems very unlikely that any measurable amount would be left in cooked commercial rolled oats.

Gas chromatographic methods have been developed for EDB by BERCK [15] and for propargyl bromide by The Dow Chemical Company [8]. These methods very likely could be adapted for residues of 0.1 ppm or less of EDB. BIELORAI and ALUMOT [11] describe a gas-liquid chromatography method for analyzing for EDB in foods. The sensitivity to EDB depends on the type of detector (40 ppm for thermal conductivity and around 4 ppm for flame ionization). No volatile substances other than EDB were found in fumigated mash, oat flakes, pearl barley, lentile, sorghum and wheat grain where EDB ranged from 15 to 1610 ppm. BIELORAI and ALUMOT [10] describe an electron-capture gas chromatography method which allows detection of ppb of CCl_4 , CS_2 , chloroform and trichloroethylene. This method should be adaptable to EDB.

Conclusions

A method to detect EDB at 0.1 ppm or less is desired which would then give the sensitivity needed to detect unchanged minute amounts of EDB and to thus ascertain related aeration and residue problems in the foods of the consumer. Assuming that such a method becomes available, a working party could be formed to obtain this data.

Carbon disulfide

What is the nature of residues in treated food?

The carbon disulfide analytical methods of DUNNING [19] and KEPPEL and MUNSEY [20] showed recoveries of 86–103 % of CS₂ from fumigated flour, wheat, rolled oats, and bread. Sensitivity of the methods appeared to be below 1 ppm. Carbon disulfide is thought to be very stable. CS₂-reaction residues were not studied. The effect of aeration of CS₂ was studied by LYNN and VORHES [21]. CS₂-treated grain under various conditions of aeration contain residues of CS₂ of less than 1 to 40 ppm at the time of sampling. MUNSEY *et al.* [18] added CS₂ to bread ingredients 10 × the residue levels usually found following fumigations and baked them into bread loaves. The CS₂ content was reduced from 10.6 and 7 ppm to less than 0.5 ppm (below the analytical sensitivity limit for CS₂). Rolled oats, containing 10 × the residue level of CS₂ likely from usual fumigation procedures, quick-cooked for one minute, reduced CS₂ 88 % from 10.4 to 1.2 ppm. Considering normal processing procedure for producing rolled oats, it seems very unlikely that any measurable amount would be left in cooked commercial rolled oats. BIELORAI and ALUMOT [10] have described an electron-capture gas chromatography method for CS₂ sensitive to ppb, although recovery of standard mixtures from the gas chromatograph was only 40–50.

Conclusions

CS₂ as such is not likely to occur as a residue in fumigated foods after normal aeration and cooking. BIELORAI and ALUMOT's method [10] may make it possible to identify CS₂ in ppb. CS₂ reaction products in food, if present, have not been accounted for.

Carbon tetrachloride

CCl₄ is used mainly for grain fumigation. Studies on wheat, oats, rough rice, corn and grain sorghum fumigated with CCl₄ show the retention of some CCl₄ in all of these grains [21]. When wheat grain was broken by milling to flour, shorts and bran, the latter contained the most CCl₄ initially, but aerated to the same levels as flour and shorts during shipping. CCl₄ residues in flour are lost upon baking into bread [1, 18]. BIELORAI and ALUMOT [10] describe an electron-capture gas chromatography method which allows detection of CCl₄ in the ppb range. In their tests, CCl₄ was not completely aerated from wheat or barley after 17 days following fumigation with relatively small dosages of CCl₄. No information seems available on the presence or absence of CCl₄ metabolites in treated grain. WILLIAMS [24] indicates that CCl₄ is only slightly metabolized in mammals. In view of this information and the known chemical stability of CCl₄, it is not likely that there are degradation products or metabolites of any significance formed while the fumigant is a residue in grain. In fact the very persistence of small amounts of unchanged CCl₄ in grain over long periods of time [19] support this assumption. Thus, it seems reasonable to deduce that further inquiry into metabolites or degradation products of CCl₄ in grain would not yield information that would be meaningful

with respect to safety. It seems more important to substantiate the existing indication that no significant amount in food prepared for human consumption.

Conclusions

The completeness of CCl_4 residue removal from human food by aeration and cooking can and should be ascertained.

Ethylene dichloride

Ethylene dichloride (EDC) was reviewed by the Joint Meeting of the FAO/WNO Committee on Pesticides in March 1965 [1]. A primary question remains concerning the nature and amount of EDC residues present in treated foods. No reaction products or metabolites of EDC have been found in grain [1] or rabbits [1, 24], however, EDC persists *per se* in treated grain and aerates rather slowly. As with CCl_4 , it does not seem that further work on possible degradates or metabolites is required, but that confirmation is needed to show the absence or presence of EDC in food eaten by humans. BIELORAI and ALUMOT [10] describe an electron-capture gas chromatography method which allows detection of certain chlorinated and other fumigants in the ppb range. This method can likely be adapted to estimate EDC residues.

Conclusions

The completeness of EDC residue removal from human food by aeration and cooking should be ascertained.

Chloropicrin

What are the nature and amount of chloropicrin residues present in treated food?

A method of analysis for chloropicrin (sensitive from 0.1 to 100 ppm) based on reduction to nitrite and coupling with coloring reagents was used by GETZENDANER *et al.* [22] who found that when dry beans and field peas are fumigated with chloropicrin at 2 and 4 pounds per 1000 cu.ft (24-hour exposure at 78–80 °F) that maximum residues in beans were not in excess of 1 ppm per pound of fumigant per 1000 cu.ft. Residues in peas were near the lower limit of detection. While most of the fumigant aired out of commodities such as field corn, peas, beans, wheat flour, breakfast food, and chicken feed, even after 30 days measurable amounts of chloropicrin residues were found. Biscuits baked from flour containing 16–147 ppm of chloropicrin contained 2–28 ppm after baking. Flour containing 3.7 ppm of chloropicrin before baking retained no measurable amounts afterwards. The possibility of residual inorganic nitrites and nitrosamines being formed in the grain from chloropicrin has been postulated [1]. Facts concerning residues other than chloropicrin *per se* are apparently not available. BIELORAI and ALUMOT [10] describe an electron-capture gas chromatography method which allows detection of certain halogenated and other fumigants in ppb. This method should be adaptable to chloropicrin.

Conclusions

A more specific analytical method than nitrites for chloropicrin may be necessary. Chloropicrin and reaction residues, if present, should be determined after proper aeration and cooking. A working party is justified only if the use of the chloropicrin in commercially treated goods is significant.

Pertinent data has been reported previously by FAO/WHO and IUPAC committees; no further progress is reported at this time on these compounds.

14 July 1967

E. E. KENAGA

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Appendix IX

Pyrethrum and Pyrethrum Synergist Residues

The problem as a whole has two main aspects:

- (1) Methods for determining the actual levels of pyrethrum and of synergist residues existing in their unchanged state in various commodities.
- (2) The nature and effect of terminal residues of pyrethrum and of synergist, such residues resulting from oxidation or metabolic breakdown, etc. The properties of these terminal residues would decide whether their quantitative determination was desirable also.

In our view the investigation of residues of original rethrans is more important than study of the nature and amount of terminal residues. This opinion is based on the fact that modification of the pyrethrin molecule (whether by cleavage, polymerization, oxidation or reduction) leads to a dramatic fall in biological activity. But we have no information on the relative importance of these two aspects in relation to synergists.

These aspects may now be considered in more detail.

(1) *Pyrethrins*

In view of the rather small quantities likely to be present, the method of choice for determining pyrethrum residues would be GLC with electron capture. It is fairly easy to resolve the four main components (Pyrethrins I and II and Cinerins I and II; the jasmolins could be neglected) and the values for each could be combined to give a figure for "total pyrethrins". A point to be remembered here is that the four esters may degrade at different rates, so that the composition of the residues would not necessarily be exactly that of the originally applied formulation. One line of investigation would be, therefore, to study the composition of residues (in terms of the four esters) in comparison with that of the unchanged formulation to ascertain if there were any preferential breakdown of pyrethrins or cinerins.

Other important studies would be on methods of extraction from commodities and methods of clean-up prior to GLC. In both cases it would be essential for the main commodities involved to be indicated, as it is likely that no one method would be universally applicable. Extraction and clean-up of residues on wheat, for example, is expected to be rather simpler than for cocoa or other fatty materials.

Synergist

Piperonyl butoxide and some other closely related synergists can be determined at trace level by colorimetric methods, of which several exist. The determination of synergist residue levels does provide an indirect approach to the pyrethrum levels, for if it is known that the original formulation was based on a given pyrethrum/synergist ratio, then the synergist residue level found enables an *upper* limit to be set to the pyrethrum residues. The actual residues may, of course, be considerably lower, since most synergists tend to be more stable than pyrethrum, and might persist after the latter had completely decomposed. Such an inferential figure for pyrethrum could be misleading, since the presence of synergist (which usually has no intrinsic toxicity) would be no guarantee of the presence of a proportionate quantity of pyrethrum. On the other hand, for some purposes such an inferential figure might be quite acceptable as it would be a maximum one.

Piperonyl butoxide and congeners might also be determined by GLC methods (although these do not respond well to electron-capture under the same conditions as do the pyrethrins). Study would be needed to find under what conditions the various synergists could be determined, the ideal being a single run to estimate both synergist and pyrethrum on the same chart.

It would need to be confirmed also that the extraction and clean-up procedures devised for pyrethrum were suitable for the synergist.

(2) *Terminal residues*

The study of the terminal residues would be more difficult, as it would be necessary to identify the various compounds resulting from oxidation, etc., or by metabolic breakdown in the particular commodity. These studies should include bioassays to determine whether the terminal residues had any insecticidal activity or mammalian toxicity. If biological activity appeared to be low, there would seem little necessity for developing further methods capable of quantitatively estimating such terminal residues.

In both (1) and (2) mention has been made specifically of "pyrethrum", but it is thought that many of the conclusions would be equally applicable to the synthetic analogues.

21 August 1967

E. M. THAIN, A. J. FEUELL

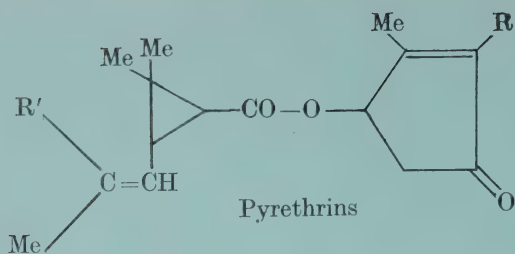
Appendix X

Rethrins and Synergists

This report is a review of the recent residue work on pyrethrins and synergists. Included are methods and amounts found in planned experiments based on use patterns. A review of work now under way on metabolic pathways is also given. The active ingredients of pyrethrum, shown in Figure 1, are known collectively as pyrethrins. Tests were designed to determine residues on foods from sprays of pyrethrins, piperonyl butoxide and MGK 264. These experiments together with the residue results were the basis for the establishment of the tolerances as food additives. Levels of terminal residues on foods exposed to pyrethrins and piperonyl butoxide from intermittent aerosols were also determined. These units are used for fly and mosquito control in restaurants. In both these cases the residues of pyrethrins and synergists were well below the tolerance levels established.

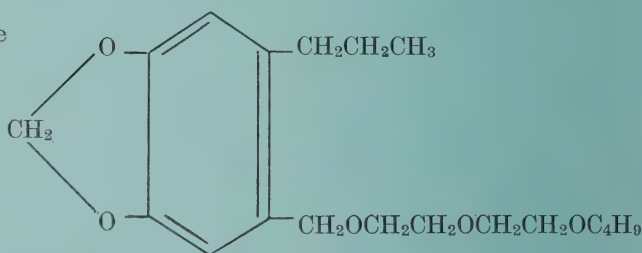
Methods of analysis

There are two methods of analysis given for pyrethrins. The GLC method has considerably better accuracy than has been available in earlier work. It is adaptable to determinations of terminal residues on food. BAKER [2] gives a biological method for pyrethrins sensitive to concentrations as low as 0.0035 ppm. BEROZA [3] and BRUCE [5] give two different but accurate methods for determination of piperonyl butoxide; the first a thin layer chromatographic method, the second a GLC method. The GLC method is sensitive to picogram quantities of piperonyl butoxide. BRUCE [5] gives a method for the determination of MGK 264. This GLC method as in the case of piperonyl butoxide is accurate in picogram quantities.



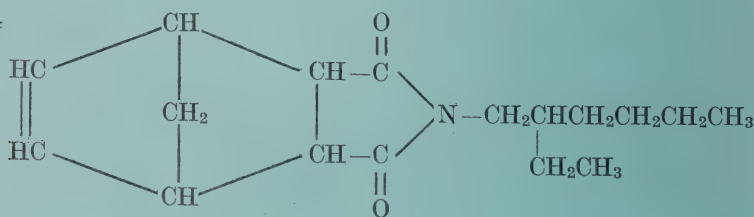
	R	R'
Pyrethrin I	$-\text{CH}_2-\text{CH}=\text{CH}-\text{CH}=\text{CH}_2$	Me
Cinerin I	$-\text{CH}_2-\text{CH}=\text{CH}-\text{Me}$	Me
Pyrethrin II	$-\text{CH}_2-\text{CH}=\text{CH}-\text{CH}=\text{CH}_2$	COOMe
Cinerin II	$-\text{CH}_2-\text{CH}=\text{CH}-\text{Me}$	COOMe
Jasmolin II	$-\text{CH}_2-\text{CH}=\text{CH}-\text{CH}_2-\text{CH}_3$	COOMe

Piperonyl butoxide



3,4-methylenedioxy-6-propylbenzyl *n*-butyl diethylene glycol ether

MGK264



N-(2-ethylhexyl)-bicyclo[2,2,1]-5-heptene-2,3-dicarboximide

Tropital

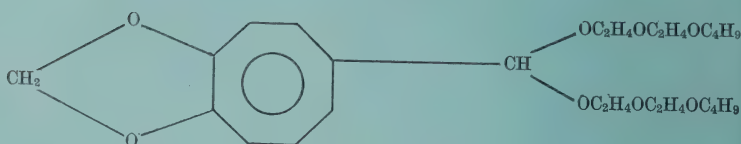


Fig. 1 Structural formulae

End products

BROWN *et al.* [4] show that upon 3 days of UV irradiation, 75% of the pyrethrins degraded. Cinerin I and II appeared more stable and lasted longer. GLYNNE-JONES [7] also showed rapid degradation of pyrethrins in sunlight. It is thought that the keto alcohol moiety degrades more rapidly than the acid moiety. The acids remain substantially the same except for a tendency toward the racemic form. Nothing appears to be known about the residue of the end products of pyrethrins degradation. There is also nothing known about the breakdown end products of either piperonyl butoxide or MGK 264. These products have both been found very stable and are recovered as such after at least a year's storage as residues on grain, paper and cotton bags.

Metabolic fate

MASRI *et al.* [8] indicate the metabolic fate of chrysanthemum acid esters to be de-esterification and oxidation upon oral ingestion. AMBROSE [1] shows that the chrysanthemumic acid is excreted in the urine in his work with rabbits. CASIDA *et al.* [6] show the work with the metabolites of piperonyl butoxide and indicate the formation of formate and then CO₂. No work is available on the study of the metabolic fate of MGK 264.

A new methylene dioxyphenyl synergist has been developed. This synergist Tropital (TM), bis[2-(2-butoxyethoxy) ethyl] acetal may be represented structurally shown in Figure 1. The work on residues and breakdown products is now in progress on this synergist.

Research now in progress and planned

There is work under way at present at the University of California, Berkeley, Cal., under the direction of Dr JOHN CASIDA on the metabolism of pyrethrins in mammals. This work is being done with radioactive pyrethrins. It is contemplated that this work will also include the metabolism of pyrethrins with and without synergists. Further studies of the metabolism of the synergist Tropital and piperonyl butoxide are now under way.

August 1967

J. B. MOORE

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Appendix XI

Chemical Nature of Terminal Residues of Organophosphorus Compounds

Since the preparation of the last report on the above subject, in November 1966, there is only a small amount of additional information to add concerning a few of the compounds discussed. There are still some unidentified metabolites from azinphos-methyl metabolism. Further work on metabolism of diazinon in plants, particularly ones with seeds of high fat content, seems advisable. With the increasing use of a greater variety of fumigants on stored grains the extensive reviews by Rowlands on this subject, with a section on organophosphorus compounds, is a welcome addition [1].

Dimethoate

One study on the metabolism of both technical and pure material by cucumbers indicated a similar total residue of < 0.5 ppm after 7 days. Small quantities of the oxygen analogue were detected, as well as an unknown cholinesterase inhibitor [2]. The variation in metabolic pathway between plants as illustrated with phosphoric acid being the main hydrolytic product from peas while the desmethyl oxygen analogue of dimethoate was predominant from corn, cotton and potato plants [3]. However, in all cases only trace amounts of dimethoate and the oxygen analogue were present 32 days after treatment. The germ in wheat is the most active decarboxylation site for dimethoate and increases greatly with moisture content [4].

Malathion

The rate of degradation (oxidative hydrolytic and decarboxylase) is affected by the moisture content and the age of the stored grain [4]. A comparison of malathion residues on treated tomatoes during commercial and home preparation indicated that commercial washing removes the majority while home-style washing removes very little. However, peeling and subsequent canning operations results in nearly complete removal of any residue [8].

Parathion

From deposits on bean leaves besides isoparathion, paranitrophenol and paraoxon unknown metabolites were noted; one intermediate between parathion and isoparathion, the other more polar than p-nitrophenol [6].

Parathion-methyl

Although no methyl paraoxon was found in carrots drenched with ^{32}P -labelled material the rate of degradation differed between varieties, the distribution being related to the amount of essential oil present [5]. Mono- and dimethylphosphate were identified from five phosphorus-containing metabolites.

Phosphamidon

The overall decomposition of both isomers proceeds at nearly equivalent rates. However, individual intermediates such as N-dealkylation of the cis isomer occurred more rapidly than the trans although the N-dealkylated trans isomer is the more toxic and active anticholinesterase [7]. Evidence was found for both the desmethyl derivative: (A) as well as the hydroxyethyl intermediate (B) as well as the metabolites mentioned previously.



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Appendix XII

Multidetector Methods for Organochlorine Pesticide Residues

At the last meeting of the Commission on Residue Analysis questions were raised as to the adequacy of the present means of identifying residues which give responses in the multidetector procedures. Subsequently the Commission was asked by interested parties to provide guidance on means of identifying residues and suggestion of a standardized method of analysis. A working group was formed to give consideration to these problems and these techniques. Five specialists actively engaged in multidetector procedures were asked to give comments on confirmatory tests and/or positive identification, sensitivities, and general ideas on methodology, advantages and disadvantages of TLC, GLC, etc., and the need for extensive experience in obtaining dependable results.

The following discussion pertains primarily to multiresidue methods for food products and would apply only generally to wildlife. In general all members stated that a system based on (a) proper extraction, (b) adequate clean-up, and (c) GLC utilizing electron capture detector was the system of choice. Only one suggested the use of TLC for routine analysis; others limited its use to confirmatory tests. Whilst there are some methods available now which can be effectively used to routinely analyze a wide variety of food products for residues of the more important organochlorine pesticides it should be pointed out that in laboratories which are concerned with studying the levels of pesticidal compounds present in a wide range of sample types of unknown treatment history, many problems remain and the position is unlikely to become completely satisfactory in the foreseeable future. As our techniques improve in sensitivity and certainty, so also does the complexity of the problems and the limitations of residue analysis become apparent. It should also be remembered that methods for the rapid screening of leafy vegetable produce may not be applicable to fruit and almost certainly will be useless for

examining wildlife tissue; compounds which are readily removed from river water may be difficult to extract from the associated bottom mud or aquatic flora and fauna.

Sampling

Here as always is a vital stage in the analytical procedure. An accurately representative sub-sample of a field of cabbages or corn is a near impossibility, while with wildlife or biopsy tissue the whole available sample may not be really adequate. Hence, sampling schemes must be chosen with due regard to the purpose for which the analyses are to be performed. Also, care must be taken not to draw too rash a conclusion on the evidence of a single sample, the representative nature of which may be in doubt. Some compromise must always be sought between that which statistical analysis shows to be desirable and that which can be followed in practice.

Extraction

It was generally agreed that "total" extraction is the most desirable when analyzing for multiple residues in samples of unknown spray history. Extraction solvents must be as efficient as possible without yielding too much co-extracted interfering material. Completeness of extraction of the residue from the sample is necessary. Recent reports have indicated certain sample types (dry forages, feeds) and residues (translocated for which conventional extraction procedures are not always effective). A multitude of extraction solvents and techniques have been reported. However, few have been tested for efficiency of extraction of a large number of compounds from a large number of different food products.

Clean-up

There was no disagreement that clean-up is necessary. Clean-up is essential for the eventual unambiguous interpretation of response to the multi-detection procedure. Present techniques could be improved, both in efficiency and speed.

End-methods of analysis

Gas chromatography has become well established as the quantitative end-method for residues of organochlorine and organophosphorus insecticides. Different members of the working party expressed various amounts of confidence in the current detectors. Each feels that research should be extended on exploring the possibility of greater selectivity. Considerably more attention should be given to purchase of the best equipment, particularly gas chromatographic, poor choices for which can result in loss of much time, money, and information. Not all detectors are equivalent with respect to stability, linearity of response, proper span between high and low levels measurable, etc., and care must be taken in choosing those which have been proven to yield the best results for residue analysis. The greater sensitivity and quantitative aspect of GLC detector over TLC appear to be one of the reasons that the TLC technique is not the end-method of choice. Kovacs [*JAOAC* 48 (1965), 311], however, worked with 5 to 10 nanograms of pesticides on TLC which is a smaller amount of residue than is reported by most authors.

Confirmatory tests, identity, and experience of analysis

In the letter asking for comments on these procedures, the need for experience was separate from confirmatory test and identity; however, most of the comments essentially imply that they are not separatable. In essence the certainty of the identity of a residue from an agricultural food product depends a good deal on the expertness, experience, and judgment of the residue analyst. This holds to a much less degree in fish, wildlife, and some environmental samples because the latter may be exposed to many industrial chemicals as well as agricultural chemicals and to the many possible alteration chemicals which can form in a "food chain" in an aquatic environment. The following views were expressed.

With a given sample analysis indicating the presence of a residue, probably the greatest difficulty, on a routine basis, lies in confirming the identity of the residue. Related to this is the situation when a substance is indicated present in the sample extract but cannot be tentatively identified as a pesticide. It is entirely possible when using chromatographic techniques for a nonpesticide substance to cause a response indicative of a given pesticide. However, a competent residue analyst will rarely report a "false positive". In cases where the positive response is significant the application of additional tests may not identify the substance but will rule out the pesticide first indicated present.

Experience and know-how of the analyst are extremely important in the analysis of samples for pesticide residues. First the work at the bench must be done with care and in a quantitative manner. But the residue analyst must be more than an excellent technician. He must understand the method in great detail. Undoubtedly, in the course of time he will be faced with new and unusual applications of a given method. Even more experience and know-how is necessary when difficult situations requiring confirmation of identity arise. The residue analyst should have a knowledge covering the span from pesticide use practices to techniques for isolating a pure fraction of the residue for infrared or mass spectrometry. He should have a good grasp of pesticide chemistry, an intimate knowledge of how a large number of compounds and foods behave with the method and a good ability for deductive reasoning.

Separation, confirmation, and positive identification are closely related. Separation as an inherent part of the determination makes possible multi-residue analyses. Separation of pesticides into groups prior to the chromatographic determination increases the qualitative capabilities of the method. Additional qualitative information may be obtained by using two or more systems with one of the chromatographic determinations, i.e. two different gas chromatographic columns. Based on findings of pesticides in foods in the United States and the availability of two gas chromatographic columns each capable of different separations, a method which makes no separation prior to GLC can be effectively used. However, this places a greater responsibility on the analyst to determine when additional GLC separation must be obtained and when separation prior to GLC must be done. With residues such as toxaphene and chlordane, separation prior to GLC must be obtained to determine if smaller amounts of other compounds such as dieldrin or endrin may be present.

Information leading to confirmation of identity can be obtained by (1) chromatography on a second GLC column capable of different separations, (2) GLC coupled with specific detectors, (3) TLC utilizing a second solvent system capable of different separations, (4) *p*-values, (5) TLC spray reagents giving specific reactions, (6) chemical derivatives or known reactions to certain chemical treatment, (7) separations achieved prior to determination,

- (8) knowledge of which compounds the method will and will not recover, and
- (9) information on spray history of the sample.

Infrared and mass spectrometry may be used providing a sufficient amount of the unknown can be isolated in pure form and the significance of the sample and residue warrant extensive effort. Polarography may find application when certain residues are indicated, and colorimetric methods which are available for some compounds may be helpful.

Knowledge of the sample's history (where this is available) and a thorough knowledge of and experience with the methodology and the particular equipment used can aid the analyst in correctly interpreting GLC responses. In many instances this competent interpretation is sufficient for the purpose of the particular study. However, the certainty of correct interpretation of a multidetection procedure cannot be obtained without further confirmatory identification.

It was completely agreed that confirmation tests are needed, as together with a knowledge what clean-up is necessary and sufficient for subsequent infrared and mass spectrometric analyses.

Organophosphorus compounds

The majority of the members favoured the inclusion of organophosphorus compounds into a multidetection procedure. Dual electron capture-flame thermionic GLC detection is already a practical reality proving very useful for combined residues of organochlorine and organophosphorus pesticides. The AOAC Official Method originally designed for organochlorine pesticides, has been expanded to include 7 parent organophosphorus compounds and it should be possible to have a single method capable of handling a number of pesticides from both these and other pesticide classes.

Research suggestions

- (1) Investigation into clean-up techniques and selective detectors (speed, effectiveness).
- (2) Use of long thin columns and better use of adsorbents deactivated with water for clean-up.
- (3) Use of solvents of as low polarity as possible for the better separation of high polarity organophosphorus degradation products.
- (4) What clean-up is necessary and sufficient for subsequent IR and MS analysis.
- (5) "Distillation" methods clean-up deserve a thorough evaluation, especially sweep co-distillation.
- (6) A greater knowledge of the capabilities and limits of the procedure is necessary. What is the precision of sampling and subsampling? How efficient and how precise is the recovery through various extraction and clean-up methods?
- (7) More research is necessary to develop practical procedures suitable for routine confirmation of identity such as procedures for the preparation of chemical alterations of the pesticide prior to chromatography.
- (8) Further work is desirable to increase sensitivity and selectivity of detection techniques (on TLC).

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Appendix XIII

Organophosphorus Pesticides Residue Analysis

The organophosphorus compounds of most immediate interest to the Commission at present are:

	Acceptable daily intake (FAO/WHO I and II)
azinphos-methyl	0.0025 mg/kg
demeton	0.0025 mg/kg
demeton-methyl sulfoxide	0.0025 mg/kg
diazinon	0.002 mg/kg
dimethoate	0.004 mg/kg
fenitrothion	—
malathion	0.02 mg/kg
parathion	0.005 mg/kg
parathion-methyl	0.01 mg/kg
phosphamidon	0.001 mg/kg

Malathion was under consideration at the last meeting and is therefore included here. Allowable daily intake levels and the tolerances likely to be derived therefrom in relation to the sensitivity of present analytical methods have been examined. Toxicologically "permissible levels" of residues may be computed from the acceptable daily intakes. For persons with a body weight of 60 kg, the following equation is applied:

$$\text{permissible level} = \text{a.d.i.} \times 60/F \text{ ppm}$$

The food factor F gives the proportion of the respective commodity in the daily food, expressed as kilograms. The FAO/WHO Working Parties recommend that the ninth decile figures of food consumed, as given in the 1955 US Household Food Consumption Survey (FAO/WHO III), should be used for the principal foods of plant origin, as indicated in Table I. The Expert Committee of the European Economic Community has proposed the following values (Dormal-van den Bruel):

fruits and vegetables (excluding potatoes)	0.4 kg
cereal products	0.3 kg
oils and fats (excluding milk and milk products)	0.1 kg

These figures are comparable in their order of magnitude with the US values.

Table II readily permits interpolations and extrapolations and provides information on the interrelationships between a.d.i., food factor, and permissible level. Since the permissible level becomes proportionally smaller as the food factor increases, prime consideration need only be given to the principle foods for an assessment of the "sensitivity" of analytical procedures in relation to the permissible levels. The permissible levels (ppm) set out in Table III might therefore be considered as the basis for further deliberations.

An acceptable daily intake value has not yet been published for fenitrothion. Since this compound is less toxic and is a weaker cholinesterase inhibitor than parathion-methyl (HOLLINGWORTH *et al.*), it can be placed in at least the same category as parathion-methyl. Tolerances are usually lower than the permissible levels so that residual analytical methods must be so "sensitive" that at least the lowest permissible levels can be quantitatively determined with absolute reliability. Therefore, the minimum re-

quirements for the lower limit of determination of the 10 compounds could be as indicated in Table IV. These limits would apply mainly to "enforcement" methods rather than to procedures used for academic studies on the behavior of a given compound on and in biological systems.

These limits apply to crops with the highest consumption rate, and for which analytical methods are primarily developed. Difficulties which may arise in the analysis of particular crops with a relatively low consumption rate are usually offset by higher permissible levels. In countries where tolerances have been established which are considerably below the permissible levels, it may be necessary to review the different methods in individual cases. However, this is only possible when tolerances already exist or are to be established. An assessment of the existing analytical methods can only be made on condition that the Commission on Terminal Pesticide Residues does not consider further requirements to be necessary with respect to the detectability of metabolites. Since multidetection systems would offer the best prospects for controlling food moving in international commerce, they should be discussed first, without, however, taking into account biological techniques and semi-quantitative methods. GLC should be given preference for analyses which are capable of simultaneously identifying and making a quantitative determination, since this technique is considerable more reproducible and in many cases operates more sensitively than "layer-chromatographic" systems. Numerous studies have been published dealing with the separation of OPs in the absence of plant extractives. These studies will not be discussed here since the authors make no reference to the possible use of their methods for analyzing residues.

Abbreviations used:

OP	= organophosphorus insecticide
GLC	= gas chromatography
TLC	= thin layer chromatography
IR	= infrared spectrometry
ECD	= electron capture detector +
TD	= thermionic detector +
MCD	= micro coulombmetric detector +
ESD	= emission spectrometric detector +
≠	= parent compound only
+	see WESTLAKE and GUNTHER

(a) McCauley describes a vacuum sublimation clean-up, followed by quantitative determination by GLC and identification by IR.

The method includes:

 diazinon, azinphos-methyl, parathion, parathion-methyl, malathion
 detector: ECD
 column: 2% neopentyl glycol adipate on 50/60 mesh Anachrom ABS
 substrates: apples, tomatoes, spinach, lettuce, cauliflower, cabbage, turnips, potatoes

Sufficient recoveries are reported, excluding, however, low levels.

Other OPs included in the study with positive results:

 carbophenothion ≠
 demeton ≠
 disulfoton ≠
 EPN
 ethion

(b) STORHERR *et al.* (1964) differentiated between:

diazinon, parathion, parathion-methyl, malathion
clean-up: Norite/MgO/Celite
column, eluted with 25% ethyl acetate in benzene
detector: not stated
column: not stated
substrates: kale, carrots, lettuce, spinach, cabbage, potatoes,
apples, strawberries

Recoveries were over 80% at the 0.1 ppm.

Other OPs included in the study with positive results:

carbophenothion \pm

(c) WESSEL has reported good recoveries at the 0.5 ppm level for OPs including

diazinon, parathion, parathion-methyl, malathion
clean-up: Mills procedure
detectors: ECD and TD
columns: 10% DC-200 on 80/100 mesh Gas Chrom Q
or Anakrom ABS
substrates: lettuce, apples

Other OPs included in the study with positive results:

carbophenothion \pm , ethion, ronnel

(d) SANS determined OPs amongst a large number of pesticides, including

diazinon, azinphos-methyl, parathion, malathion,
following fractionation from Florisil and chemical conversion
clean-up: not reported
detector: ECD
columns: 5% DC-11 on 60/80 mesh Chromosorb W (non acid
washed)
and 5% QF-1 on same, HMDS-treated
substrates: alfalfa, carrots, corn, onions, tobacco, radishes, tur-
nips

Experiments were carried out at 10 μ g levels. Limits of detectability in terms of ppm are not reported.

Other OPs included in the study with positive results:

carbophenothion \pm
dicofol
disulfoton \pm
ethion \pm
Nemacide
phorate \pm
trichloronate (Bayer 37 289)

(e) MÖLLHOFF, in the referee's laboratory, differentiated between parathion type compounds:

parathion, parathion-methyl, fenitrothion
clean-up: Florisil/benzene
detector: ECD
columns: 5% QF-1 on 60/80 mesh Chromosorb W, HMDS-
treated (SE-30, DC-11, E-301 for comparison)
substrates: apples, cabbage, lettuce, carrots, onions, potatoes

Recoveries are satisfactory at the 0.1 ppm level.

Other OPs included in the study with positive results:

chlorthion

trichloronate (Bayer 37 289)

(f) NELSON I, in following up on his own previous studies, investigated 16 OPs including

a) diazinon, b) parathion, c) parathion-methyl, d) malathion

Satisfactory recoveries are given for

a) at 0.1 ppm, b) at 0.1 ppm, c) at 0.25 ppm, d) at 0.1 ppm

Dimethoate and azinphos-methyl gave good recoveries with a modified procedure (NELSON II).

clean-up: Mills-Onley-Gaither

detector: MCD

columns: 15% DC-200 on 30/60 mesh Chromosorb P (multi-linear temperature program)
or 10% QF-1 on HMDS-treated 60/80 mesh Chromosorb W

substrates: oranges, apples, strawberries, plums, lettuce (for a);
plums, lettuce, apricots (for b);
apples, plums, lettuce, cabbage (for c);
apricots, peaches, grapes, lettuce (for d).

Other OPs included in the study with positive results:

carbophenothion \pm , Delnav, disulfoton \pm , EPN, ethion, fenthion (Baytex) \pm , ronnel, sulfotepp

(g) BACHE and LISK I, studying 18 OPs reported recoveries of more than 80% for

diazinon, dimethoate, parathion

clean-up: varying

detector: ESD

columns: 5% Dow Corning high vacuum silicone grease (ethyl acetate soluble)
or SE-30 on 80/100 mesh acid washed Chromosorb W

substrates: grapes (diazinon), lettuce (dimethoate, parathion), alfalfa, milk (dimethoate)

Recoveries were checked in the 0.1–0.6 ppm region (not consistently). However, relative retention times are not stated.

Other OPs included in the study with positive results:

disulfoton \pm , ethion, ronnel

(h) Chemagro Corporation I, in a method for determination of disulfoton residues, report relative retention times for 14 OPs which would allow separation of

diazinon + parathion-methyl from parathion + malathion and azinphos-methyl

clean-up: carbon column with a 30/70 chloroform/acetone mixture as eluant

detector: TD

column: 10% DC-200 and 1.5% QF-1 on 80/100 mesh Gas Chrom Q

Details on recoveries are not given, since all compounds were only checked for possible interference with the analytical method.

Other OPs included in the study:

carbophenothion \pm
DEF
Delnav
demeton + metabolites
EPN
ethion
malaoxon

These few examples from more recent studies demonstrate that GLC could well be recommended for multidetection of OPs including many of these under consideration here. Column and detector conditions would only have to be uniformed in order to make common use of the experience accumulated thus far. For this purpose, the extensive studies of BURKE and HOLSWADE, covering 85 pesticides (including 21 OPs) could be evaluated. These authors employed a mixture of equal portions 15% QF-1 on 80/100 mesh Gas Chrom Q and 10% DC-200 on 80/100 mesh Gas Chrom Q, using ECD and MCD.

There is also need for a uniform clean-up. SAMUEL, and SAMUEL and HODGES in evaluating screening methods for OP and organochlorine residues, report quantitative recoveries for several OPs using an adsorbent mixture and/or Florisil columns for clean-up of various crops. In the referee's laboratory, excellent recoveries were found with approx. 30 OPs including many metabolites, using an Al_2O_3 column (activity grade V) and chloroform/carbon tetrachloride (1:1 v/v) as eluant. Further recovery studies are in progress. These systems appear to be worthwhile for future testing. Sweep co-distillation also opens promising prospects. STORHERR and coworkers recently extended their pertinent contributions to the determination of diazinon, azinphos-methyl parathion, parathion-methyl, and malathion in milk and edible oils down to 0.1–0.01 ppm (except azinphos-methyl), using GLC as the final step (WATTS, STORHERR *et al.*, 1967; cf. modification by HARTMAN).

At all events, suitable combinations of the main parameters, clean-up, gas chromatographic column and detector must still be found. The lower limits of determination will, in general, meet the requirements presented in Table IV. The published results on the GLC of OPs very probably represent only a small percentage of the results meanwhile available all over the world, especially considering that work on this field has received a very great impulse since the introduction of the TD. Residue laboratories which have worked on the GLC of OPs should be asked to make their experience available to the Commission. It is trivial but nonetheless cannot be sufficiently emphasized that in view of the large number of OPs available on the world market, as well as their metabolites, it is extremely difficult to make clear identifications of individual components as long as additional possibilities of identification are not exploited. It must, therefore, be borne in mind that the methods of determination referred to above may fail in the presence of other OP residues.

Special methods are available for all of the compounds under consideration, although these procedures are not necessarily specific.

Phosphamidon

and its metabolite, desethylphosphamidon, have been determined, after paper chromatography, by elution of the spots and determination of P by the phosphomolybdenum blue method (ANLIKER and MENZER). Although the authors claim that the limit of detection is 0.5–1 μg , recoveries are

reported for various crops in the region of several ppm only. Automated cholinesterase inhibition technique can be employed down to approx. 0.05 ppm (VOSS and GEISSBÜHLER). An additional TLC step offers a high degree of specificity. Recoveries for various crops are over 80%. The "iodoform procedure", developed for Bidrin (STEVENS and VAN MIDDELEM), can be applied to the determination of phosphamidon with an ECD since it is specific for methylvinyl phosphates. The procedure, however, seems to be difficult and was not sufficiently reproducible in other laboratories. It is, however, capable also of determining the metabolite.

Phosphamidon residues in olive oil are determined by a total phosphorus method and (VASSILOU *et al.*). A total phosphorus has also been described for apples (BREWERTON). Both methods are capable of determining residues down to approx. 0.1 ppm.

Diazinon

Geigy have reported a colorimetric (Geigy I) and a gas chromatographic (Geigy II) method, the latter using either ECD or MCD. The colorimetric procedure is based on methylene blue formation and is specific owing to the weakly basic properties of diazinon. Both methods are suitable for a broad variety of crops; the lower limit of determination is 0.05 and 0.02 ppm, respectively. See azinphos-methyl for determination of surface residues.

Azinphos-methyl

Besides the two commonly used colorimetric procedures (MEAGHER *et al.*, MILES), Chemagro II has developed a gas chromatographic method, using a 15-inch column (5% DC-200 on 70/80 mesh DMCS-treated Chromosorb G). The method has been checked with 100% recoveries down to 0.4 ppm on alfalfa. The method of MEAGHER *et al.* has been subject to criticism by Cox I (on its length), and attempts have been made to increase its sensitivity by concentrating the resultant color by extracting into chloroform (GEORGE). It was, however, included as First Action in the "Official Methods of Analysis" of the AOAC (10th ed., 1965). Both colorimetric methods are sensitive to approx. 0.1 ppm (MEAGHER *et al.*; FREHSE, 1966/67, unpublished [MILES does not state recoveries below 1 ppm]).

BLUMAN's "short method", as studied by Cox II, utilizes MEAGHER's colorimetric principle, but determines surface residues only. So does the procedure of BRODERICK *et al.*, based on total phosphorus, for azinphos-methyl and diazinon on whole fresh fruit. AOAC is at present attempting to combine the best features of these methods (RAMSEY). Residues in milk can be determined down to 0.005 ppm by a spectrofluorimetric method [ADAMS, J.M. / ANDERSON, C.A.: *J. Agr. Food Chem.* 14 (1966), 53-55].

Demeton

A total phosphorus method is available which is capable of determining the parent compound isomers as well as their sulfoxides and sulfones (ZWEIG, Vol. II; Chemagro III). Plant blanks for various crops vary between 0.07 and 0.25 ppm. Recoveries studied mainly in the range between 0.6 and 1.5 ppm, are reported to fluctuate from approx. 60% to approx. 120% with an average of about 80% (Chemagro III). These residues have been separated for qualitative determination from many other registered (USA) cholinesterase-inhibiting pesticides by paper chromatography (ADAMS *et al.*).

Since 3 of the 5 possible metabolites have identical R_F values, identification should include an oxidation step to yield the respective sulfone(s) which can be quantitatively measured by I.R. at 7.55μ (GIANG and SCHECHTER).

Demeton-(thiol)-sulfone can also be determined by GLC using a TD (Chemagro I, see p. 140). Recoveries for corn, soybeans, sugarcane and sugarcane products are in the 100 % range at 0.1 ppm.

AOAC is studying a gas chromatographic method including the metabolites (McKINLEY, RAMSEY).

Demeton-S-methyl-sulfoxide

The method based on total phosphorus as described for demeton is applicable, with minor alterations, also to this compound and its metabolite, the sulfone (Chemagro IV). Identifications could underlay similar considerations as for demeton. Pertinent experience has been accumulated using I.R. techniques following permanganate oxidation (FREHSE), and TLC (FREHSE, 1967, unpublished).

Another total phosphorus method for demeton-methyl residues is based on a clean-up by chromatography on a column of desactivated Al_2O_3 (grade V). Recoveries are between 80 and 100 % down to 0.2 ppm for various crops; blank values range from 0.05 to 0.2 ppm; additional identification for enforcement purposes is necessary (FREHSE, 1966, unpublished). Demeton-methyl is also included in AOAC's GLC studies for demeton (which see).

Dimethoate

Many colorimetric methods, based on various principles, are available (SMART I). For recent developments see GEORGE *et al.* (colorimetric, methylamine basis), BACHE and LISK II (GLC with ESD), MITSUI *et al.* (colorimetric, thioglycolic acid basis). It is suggested that the final report of the Joint Dimethoate Residues Panel established in the United Kingdom be awaited for further consideration. The method (cf. SMART II) will include a simple clean-up, followed by total phosphorus determination, including identification by TLC and/or GLC. The lower limit of determination is about 0.2 ppm for fruits and vegetables.

Parathion and parathion-methyl

The classical colorimetric procedure after AVERELL and NORRIS has, in general, proved to be satisfactory for most purposes. It was adopted as Final Action by AOAC (Official Methods, 10th ed.). The method, however, is based on stripping solutions, which might be subject to fundamental objections. Moreover, interferences may be encountered with particular crops. GLC procedures starting from real macerates should be preferred. Numerous approaches have been reported (cf. MÖLLHOFF). No further action appears necessary.

Fenitrothion

can be determined according to the AVERELL-NORRIS procedure with slight modifications (NIESSEN and FREHSE for crops in general, HORLER for barley). Furthermore, determinations on the basis of colorimetric evaluations of the 3-methyl-4-nitrophenolate have been reported (KOVÁČ and SOHLER, MIYAMATO *et al.* for bananas, FRANZ and KOVÁČ for milk). Recoveries are sufficient down to 0.1 ppm (NIESSEN and FREHSE, KOVÁČ and SOHLER) and 0.05 ppm in the milk method.

Just as for the parathions, GLC methods should be preferred for fenitrothion. Three procedures using ECD have been described:

- DAWSON *et al.* used 0.25 % Epikote 1001 and 2.5 % silicone elastomer E-301 on 100/120 mesh Celite. A recovery of 95 % (? ppm) is given for cocoa beans, employing "liquid" clean-up steps.
- MÖLLHOFF (see p. 139) obtained good recoveries for various crops down to 0.1 ppm level.
- HORLER used 0.3 % Epikote 1001 and 3 % Apiezon L on 100/120 mesh Celite.
A recovery of 88 % is given for barley at the 1.5 ppm level.

The present methods would have to be checked for detectability of the oxygen analogue which is formed on plants in very minute amounts.

Malathion

The well-known colorimetric method has been adopted as First Action by AOAC (Official Methods, 10th ed.) for firm fruits, vegetables, and soft or wet materials in general. Firm fruits are stripped, and other materials are macerated before further clean-up. For aged residues on fruits, maceration appears advisable (KOIVISTOINEN *et al.*). YAMAUCHI also suggests maceration of vegetables, fruits, and rice, hydrolyzing with ethanolic potassium hydroxide. Compounds yielding dimethyl dithiophosphate by alkali hydrolysis interfere with the analysis.

These methods are sensitive to 0.1–0.2 ppm, yielding recoveries of above 60 %. The same working principles, with minor modifications based on procedures according to the British Analytical Panel (1960), EPPO (1964), and ALESSANDRINI and LEONI (1965), are suggested for determination of malathion in cereals (see FAO for respective references and details).

The AOAC referee (RAMSEY) has suggested that the studies on the First Action method be continued.

Conclusions

For most of the compounds under consideration, multidetection and special methods are available. Multidetection procedure must be uniformed so as to cover as many compounds as possible. In particular, and this applies to OPs much more than to other groups of compounds, uniform clean-up methods must be agreed upon as long as "general" methods are being aimed at.

The sensitivities of the available methods appear sufficient in the light of the permissible levels and possible tolerances deriving therefrom. As an exception, phosphamidon might pose certain problems in this respect.

Decisions on toxicologically significant metabolites should be reached before evaluations are made on the suitability of analytical methods to detect these compounds.

August 1967

H. FREHSE

Table I Ninth decile food consumption values—U.S. 1955 (FAO/WHO III)

Vegetables fresh (total)		0.37 kg
potatoes, incl. sweet	0.2	
Fruits, fresh (total)		0.45
tree fruits	0.23	
fresh, various	0.2	
citrus	0.23	

Tomatoes	0.06
Pickles, olives, relishes	0.03
Nuts	0.02
Cereals and cereal products (FAO)	0.4

Table IV Minimum requirements for lower limit of determination

Phosphamidon	less than 0.1
Diazinon	less than 0.2
Azinphos-methyl	0.2
Demeton	0.2
Demeton-S-methyl-sulfoxide	0.2
Dimethoate	less than 0.5
Parathion	0.5
Parathion-methyl	less than 1.0
Fenitrothion	less than 1.0 (?)
Malathion	1.0

Table II Permissible levels based on 60 kg body weight calculated for various acceptable daily intakes and food factors

Food factor	a.d.i.					
	0.001	0.002	0.0025	0.004	0.005	0.01
0.05	1.2	2.4	3	4.8	6	12
0.1	0.6	1.2	1.5	2.4	3	6
0.15	0.4	0.8	1.0	1.6	2	4
0.2	0.3	0.6	0.75	1.2	1.5	3
0.25	0.24	0.48	0.6	0.96	1.2	2.4
0.3	0.2	0.4	0.5	0.8	1.0	2
0.35	0.17	0.34	0.43	0.69	0.86	1.71
0.4	0.15	0.3	0.38	0.6	0.75	1.5
0.45	0.13	0.27	0.33	0.53	0.67	1.33
0.5	0.12	0.24	0.3	0.48	0.6	1.2
0.6	0.10	0.2	0.25	0.4	0.5	1.0
0.7	0.09	0.17	0.22	0.34	0.43	0.86
0.8	0.08	0.15	0.19	0.3	0.38	0.75
0.9	0.07	0.13	0.17	0.27	0.33	0.67
1.0	0.06	0.12	0.15	0.24	0.3	0.6

a.d.i. expressed as mg/kg body weight, food factor as kg, permissible levels as ppm

Table III Possible permissible levels, ppm

	Phosphamidon	Diazinon	Azinphos-methyl, demeton, demeton-S-methyl-sulfoxide	Dimethoate	Parathion	Parathion-methyl (fenitrothion ?)	Malathion
Vegetables, fresh, total	0.16	0.33	0.41	0.65	0.8	1.6	3.2
Fruits, fresh total	0.13	0.27	0.33	0.53	0.67	1.3	2.7
Tree fruits	0.26	0.52	0.65	1.05	1.3	2.6	5.2
Fruits, fresh various	0.3	0.6	0.75	1.2	1.5	3	6
Citrus fruits	0.26	0.52	0.65	1.05	1.3	2.6	5.2
Cereals, cereal products	0.15	0.3	0.38	0.6	0.75	1.5	3

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Appendix XIV

Organomercury Residue Analysis

(1) *Agricultural use of mercury*

Mercury compounds have been used in agriculture for a long time. Three principal types of mercury compound are of agricultural interest, alkylmercury compounds, alkoxyethylmercury compounds and arylmercury compounds. In some areas arylmercurials are used only as fungicides for the preservation of wet pulp; although an industrial use, this is here considered with agricultural uses.

(2) *Other environmental sources of mercury*

In some countries the presence of small amounts of mercury in biological samples has become a matter of great public interest. Although mercury compounds are in use as pesticides, the content of mercury now found in wildlife and in some samples of food must not unrestrictedly be classified as residues of pesticides. The reason for this statement may be summarized as below:

(a) Mercury is a naturally occurring element widely spread in nature usually in low concentrations. The mercury content in the air is approx. 20 ng/m³; in rain water about 200 ng/l.

(b) Metallic mercury finds a variety of technical usages; during manufacture or especially on the disposal of worn or used products such as electrical relays, an unknown quantity of metallic mercury is introduced into nature.

(c) Soluble inorganic salts of mercury are also used industrially (on a reduced scale) and thus some mercury will be introduced into sewage.

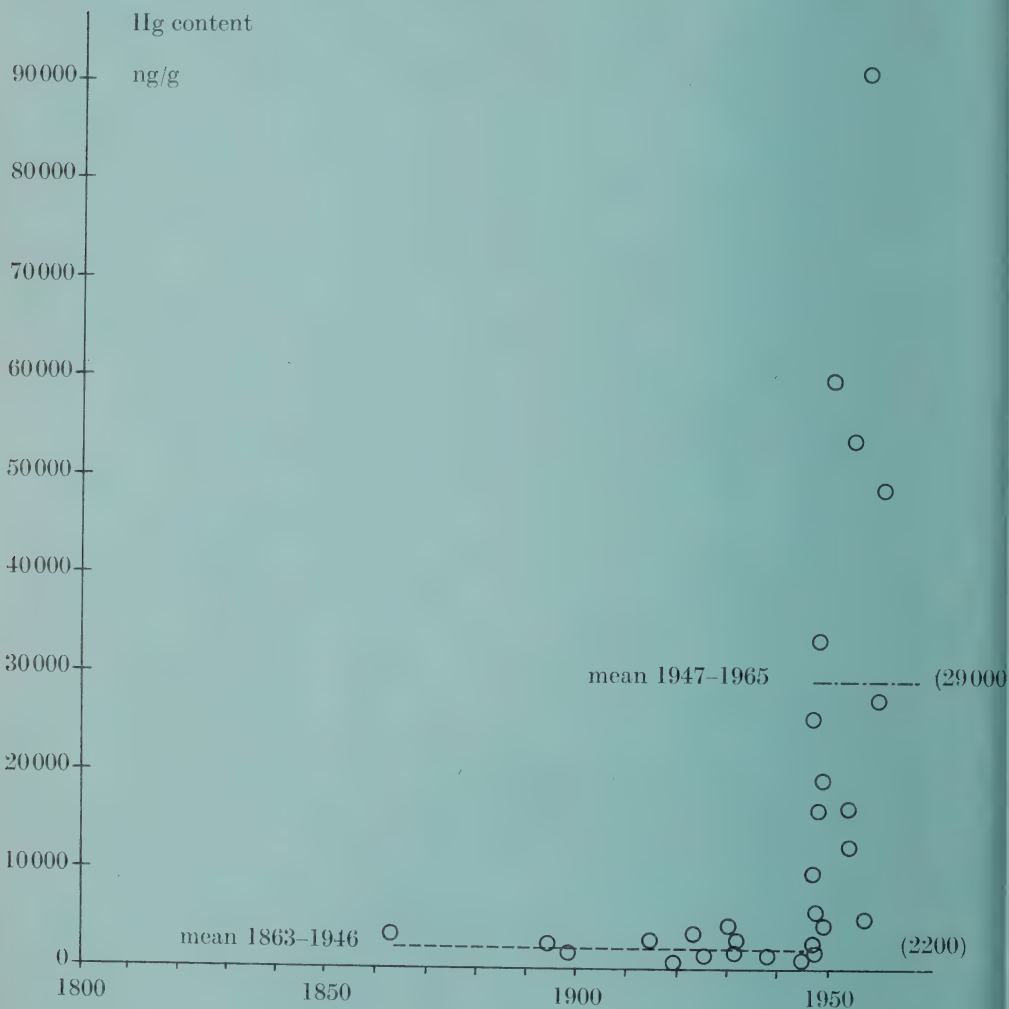
(d) In chemical industries electrodes of mercury are in use and vapours of mercury will accompany the waste gases through chimneys into the air. In Sweden it has been estimated that in 1964 the chlorine industry adds approximately 5 tons of mercury into the air and another 5 tons to the water; this can be compared with 3.5 tons of phenyl mercury as waste from the pulp industry (+ 0.5 tons from the burning of newspaper) and 4.5 tons of methyl mercury as seed dressing. (The use of alkyl and phenyl mercury is now banned in Sweden.)

(e) Since most minerals, fuels and soils contain trace amounts of mercury, heating of these materials on a *large* scale will serve as a source for the contamination of mercury in nature.

(f) The same might be valid for extraction processes, e.g. flotation of ore using reagents of complex forming properties.

(g) Non-mercury containing pollutants with complex forming properties may be able to convert mercurial minerals into a biologically receptable form.

(h) There are recent indications of the presence of a naturally occurring alkylation process able to convert inorganic mercury into organomercury.



(3) Contamination of mercury in nature

During recent years a large number of biological samples have been analyzed in Sweden for mercury; mainly total mercury. Unexpectedly high contents of mercury have been found especially in wildlife, up to 8 $\mu\text{g/g}$ in a pike.

However, with a few exceptions samples of food collected on the Swedish market were found to contain less than 50 ng/g. [Detailed report on the Swedish investigations, see "The Mercury Problem", Symposium in Stockholm, January 1966, in press.]

In Canada a very large number of samples of human hair have been analyzed for mercury and some other trace elements. There were found only few hairs with high content of mercury; of the few foreign hairs examined those from Japan showed higher values. These findings have created an interest in Japan for a similar survey. Finally, highly contamination samples have been analyzed in Japan after the Minimata accident. Although very few cases are reported—including those from Minimata—where intoxications of mercury have occurred, Swedish investigations have proved that the level of mercury has increased after 1940–1950. Several examples in the Swedish report support this statement; see also Figure 1 demonstrating mercury contents of marrow of goshawk feathers in a Swedish museum collected during the period 1850–1965.

Fig. 1 Mercury content of goshawk feather marrow: WESTERMARK and JOHNELS, neutron activation analysis on 0.2 g

(4) *Toxicology*

Whilst toxicological decisions are not the immediate concern of IUPAC, the limits proposed by toxicologists are of fundamental importance to the chemist when considering the appropriate analytical methods to be used. In the case of mercury it has been erroneously understood by scientists that WHO has recommended a maximum level in food of 50 nanograms Hg per gram. It was made clear at the IAEA/FAO Expert Meeting on Mercury Contamination in Man and his Environment (Amsterdam, May 1967), however, that no such recommendation has been officially issued by WHO. An FAO working paper (November 1966) summarizes the position thus:

"The toxicity of mercury and its compounds has been considered by BIDSTRUP ['Toxicity of Mercury and its compounds', Elsevier, 1964] as of 0.1 ppm equivalent to 0.005 mg/kg body weight per day for phenylmercury acetate was unacceptable to the Joint FAO/WHO meeting in 1963 as a no-effect level for the rat. ['Evaluation of the Toxicity of Pesticide Residues in Food', FAO, Rome, 1964.] It was further pointed out that, even if the customary safety factor were applied, the acceptable daily intake for man so calculated (0.00005 mg/kg body weight) was tantamount to zero and it was concluded that it was unable for any increase in intake of mercury including phenylmercury salts, by the general population. No recommendations have been made for acceptable daily intakes of the mere toxic alkylmercurials."

In Sweden the National Institute of Health has recently accepted 1 μg Hg/g temporarily as a maximum level in fish to be used for consumption. Since it recently has been indicated that most of the mercury present in biological samples exists in an alkylated form (shown in fish), the position should be reconsidered. Moreover, having regard to the natural occurrence of mercury and the biological alkylation processes of this element, any discussion on a no-significance level of mercury in food is unrealistic.

(5) *Analytical considerations*

There was formerly generally considered to be a marked chemical difference between the mercury pesticides and other types of mercury present in nature or in technical use; the former alone being organometallic compounds. Since

organomercury was regarded to be unstable in nature only analytical methods for the determination of total mercury were used to determine residues of mercury pesticides. In view of recent discoveries, these assumptions are not correct. A true picture of the contamination of mercury in nature will only be obtainable by the use of several more specific analytical methods, some of which are discussed below. It is anticipated that every analytical method will have its specific limitations.

(a) Neutron activation analysis (NAA)

This method of analysis is the one which has been used most frequently in the modern studies of mercury content in all kinds of samples with the exception of air. In combination with chemical methods (after irradiation) sensitivities below 1 ng Hg/g can be reached. For direct measurement of the irradiated sample the limit of detection is of the order 10–100 ng/g. However, from the biological point of view the non-destructive nature of NAA is not particularly important. Gold is the only element which interferes with the determination of mercury. However, using modern instrumentation this interference can be allowed for. It is in the nature of NAA to record the total content of mercury, independent of chemical form of mercury present in the sample. For some types of analysis this is an excellent feature of NAA. However, in other cases it is obvious limitation of the method since the mercury content of biologically inactive suspended materials in a biological sample will also be recorded; this can be overcome by the use of chemical methods of pre-treatment (including all types of separation methods) although this will certainly be found to be an expensive alternative to other more specific methods of analysis. In some countries an excellent scheme of service has been built up for NAA of mercury and a great experience has been gained in these laboratories at the low-level analysis of this element. The charge for each analysis is usually less than \$20, and even for the analysis of large series the use of this service will be found to be a more favourable than the alternative of equipping a laboratory with a reactor.

(b) Atomic absorption

This method of analysis is mainly suited to trace analysis of mercury. When using a standard instrument and a cell instead of a flame the sensitivity is in the order of 10 ng, a figure which certainly can be improved. At present there are only few reports where atomic absorption methods have been used for mercury and thus there is not available the same experience as in case of NAA. When the acceptable levels of mercury have been reconsidered by the toxicologists it will very likely be found that the sensitivity of the standard instruments of atomic absorption will be sufficient for most types mercury analysis. However, methods of cleaning-up, and reduction have to be elaborated. Furthermore, cross-checks with the method of NAA are highly desirable. Special instruments applying the principle of atomic absorption have been developed, e.g. in Canada. The sensitivity of these instruments is sufficiently high for the determination of the natural levels of mercury in air (20 ng/m³). Such instruments can be carried by aircraft (helicopters) and have been used for the determination of mercury profiles around factories and other sources of mercury contamination. The results of these Canadian investigations will be of great importance when considering the industrial contributions to the contamination of mercury in nature.

(c) Colorimetric methods

The traditional methods of mercury analysis belong to this group, especially when dithizone is used as a reagent. Since many elements are known to interfere at low-level analysis of mercury this method has got a bad reputation

among some chemists. For routine analysis on a large series of defined types of samples this inexpensive type of analysis will certainly find great use. However, cross-check with other methods of analysis should be made. Furthermore, the extract of the complex of mercury dithizone might be analyzed by the more specific method of atomic absorption when elaborated methods of combustion and reduction are available.

(d) Liquid chromatography and related methods

These methods will find their use mostly at selective separation studies of different types of mercury metabolites in biological samples. The mild conditions under which the separations are performed will be of great value when applying biochemical aggregates to which the mercury compounds are weakly bound. Since many metabolites are of ionic type, electrophoresis and ionic exchange methods should also be considered; also gel filtration. Furthermore, thin layer chromatography, as in most forms of residue analysis, is an excellent method of cleaning up the sample before using other methods of analysis.

(e) Gas Chromatography (GC) and mass spectrometry

Gas chromatography in combination with electron capture detector is found to be a highly sensitive method for determination of volatile organomercury compounds. Methyl mercury compounds can be detected down to 10 pg and (although less sensitively detected) phenyl mercury bromide has recently been found to pass a GC-column unchanged. As with most kinds of electron capture detectors, the parameters to obtain linear response must be carefully examined and controlled. If this is done, GC offers an excellent way for routine analysis of biological samples containing alkyl mercury. Methods of cleaning-up the sample before GC analysis are of importance to avoid "ghost peaks", etc. More experience has to be gained in the use of these methods of cleaning-up. However, by applying a scanning mass spectrometer as a GC-detector it is easy to identify the fractions containing mercury, to the specific isotopic pattern of naturally occurring mercury. Recent improvements of mass spectrometry such as peak matching when used in this way will provide a new tool for metabolic studies.

(f) Other analytical methods

When studying the contamination of mercury in nature any reliable, specific method of separation or identification is of interest. It is to be hoped that methods other than those mentioned above will also be found useful, e.g. infrared spectroscopy on micro samples.

(6) Conclusion

The contamination of mercury in nature seems to be due to a complex series of factors, one of them being the use of mercury-containing pesticides. The complex is of great scientific interest and a further knowledge of the factors involved are of importance for a full understanding of the distribution of mercury residues in man and his environment. The treatment of the complicated problems will require the fullest cooperation of competent scientists from a variety of fields. It is strongly recommended that these studies are made in international collaboration under the supervision of international agencies (see, for example, the joint recommendations to be issued by FAO/IAEA). It is particularly important that a series of reports should be obtained on the levels of mercury from those countries where the use of alkyl

and aryl mercury have recently been banned. Such information will be of benefit to those countries where the use of the mercury pesticides is unavoidable in agriculture.

July 1967

G. WIDMARK, Stockholm

Appendix XV

Fumigant Residue Analysis

(1) Analytical requirements

Schemes of analysis cannot be discussed without brief reference to the nature and importance of the various terminal residues. The number of fumigants in common use today for the disinfestation of foodstuffs entering international trade are few: methyl bromide, ethylene dibromide, ethylene dichloride, carbon tetrachloride, ethylene oxide and phosphine (derived from tabletted preparations) are the most important and chloropicrin, carbon disulphide, hydrogen cyanide and acrylonitrile may occasionally be used. The majority of these compounds are highly volatile and the amount of the original fumigant present in the foodstuff at the end of treatment has been shown to diminish during subsequent storage, handling and processing. Health authorities now demand additional evidence on the rate of elimination of these volatile residues in different circumstances. This information is best obtained in carefully controlled trials simulating normal practical conditions and each analytical method employed should be the subject of rigorous checks to ensure that it will determine in its entirety the amount of the particular residue sought. This is of more importance than the achievement of the highest possible sensitivity of detection. In fact, the lower the content of residual material which it is sought to determine the greater is the difficulty of establishing with confidence that a high percentage recovery of this residue can be obtained. Certain of the fumigants produce reaction products which are considered to have toxicological significance and analytical methods for these are equally required.

In the investigations just discussed known compounds are being determined. A more complex problem faces the analyst required to detect and determine fumigant residues in foodstuffs the treatment of which is unknown. He requires ideally, a single, simple extraction procedure which will remove quantitatively the volatile residues of any of the commonly used fumigants which may be present. Aliquots of the extract can be subjected to a series of analytical procedures, but again, a simple procedure capable of identifying and determining all, or a majority, of these compounds would be of great convenience. Gas chromatography offers the best hope of achieving this ideal and valuable progress has recently been made in this direction. The following notes draw attention to some recent investigations of fumigant residues and developments in analytical procedures.

(2) Ethylene dibromide (EDB) residues

This fumigant is of special concern because of the marked persistence of residues of the fumigant itself in foodstuffs. Very little reaction occurs. A very comprehensive programme of work on the effect on animals of feed fumigated with EDB has been carried through between 1961 and 1965 at the Hebrew University, Rehovot, Israel, and a final report by Prof. A. BONDI and

Dr E. ALUMOT has been presented. Parts of the work have been published elsewhere. In the course of this work a variety of oil seeds, cereals, dried fruits and animal feeds were fumigated with EDB and the rate of loss by airing was followed by determining total bromine, using 2% KOH for hydrolysis (OBOMUCHI and BONDI, 1955). The steam distillation/benzene extraction method of KENNETT and HUELIN (1957) was used for direct determination of free EDB. Later a gas chromatographic method with thermal conductivity detector was used to determine the EDB in the extract (BIELORAI and ALUMOT, 1965). The same authors employed a similar procedure for determination of a fumigant mixture (see paragraph 6a, below). HEUSER and SCUDAMORE I) have determined EDB in flour and whole grain by cold extraction with an acetone/water mixture followed by gas chromatography using flame ionisation detector (see paragraph 6c, below).

(3) *Ethylene oxide (EO) residues*

Since the identification by WESLEY, ROURKE and DARBISHIRE (1965) of ethylene chlorohydrin (ECH) in foodstuffs treated with ethylene oxide, formed by its reaction with naturally occurring chlorides, there is considerable interest in the determination of this substance as well as of residues of the unreacted EO in foodstuffs which have undergone fumigation or sterilization with this gas. In a similar way propylene chlorohydrin is produced during treatment with propylene oxide. WESLEY *et al.* recovered ECH from recently treated foodstuffs by steam distillation of an aqueous slurry, estimating the amounts extracted by chemical analysis and by gas chromatography (using a flame ionisation detector). HEUSER and SCUDAMORE I have concluded from their experiments that a small proportion of any free EO present at the time of steam distillation of a flour suspension would then be converted to ECH. On the other hand the steam distillation gave only very incomplete recovery from flour of added ECH. Their method of cold extraction with an acetone/water mixture appears to give efficient recovery of both ECH and EO (see paragraph 6c, below). RAGELIS, FISHER and KLIMECK (1966) have studied the formation of ethylene and propylene chlorohydrins in flour and pepper. They used an ether extraction technique giving 76–80% recovery and followed with a clean-up procedure before determination by gas chromatography. They obtained further characterization by IR and NMR. Other workers who have recently determined the residues left after treatment with ethylene oxide (but without investigating the formation of chlorohydrin) are ADLER (1965) and KROLLER (1966).

(4) *Methyl bromide*

The considerable amount of information which continues to be published on the amounts of inorganic bromide left as a residue after fumigation with methyl bromide appears to be unrelated to any real toxic hazard. It follows from the existence in several countries of legal tolerance limits for bromide resulting from fumigation. Of more immediate interest is the development of more sensitive methods for determining any unreacted methyl bromide. Although investigation may confirm present expectations that this disappears from fumigated foodstuffs within a few days by aeration or reaction, so that it is unlikely that such residues will be present in foodstuffs passing between countries, public health analysts may still feel the need for methods to check that adequate time has been allowed or suitable treatment applied between fumigation and offer for consumption. Little work appears to have been done on the direct determination of residual methyl bromide, but the procedure of HEUSER and SCUDAMORE II involving cold extraction with an

acetone/water mixture followed by gas chromatography (see paragraph 6c, below) seems to offer a convenient method of adequate sensitivity.

(5) *Residues after fumigation with Phostoxin*

This tabletted fumigant material consists of aluminium phosphide admixed with the fire-suppressing chemical, carbamate and a small proportion of paraffin wax. Phosphine gas is evolved by reaction of the material with atmospheric moisture. After a treatment each tablet leaves a flocculent powder, which, if undisturbed, may contain several per cent of the original aluminium phosphide undecomposed. If the tabletted fumigant is allowed to come into contact with the foodstuffs and if the powdered residue is not effectively removed by subsequent processing, then the undecomposed aluminium phosphide constitutes the main, perhaps the only, residue problem with this fumigant since it appears that any phosphine gas retained by bulks of foodstuffs is rapidly lost during airing. MAYR and HILD (1964) have carried out a very extensive series of experiments in the Degesch laboratories in Frankfurt (manufacturers of the fumigant) designed to demonstrate the absence of reaction with the foodstuff and to confirm the rapid disappearance of residual phosphine by natural aeration following fumigations under commercial conditions. In small-scale laboratory tests they recovered usually 99 to 100 % of the phosphine calculated from the weight of added fumigant. Phosphine was determined by reaction with mercuric chloride followed by potentiometric titration. This method has also been used for investigations in the Pest Infestation Laboratory, Slough, but a method developed by HESELTINE (1963) is preferred for amounts of phosphine. This is based in part on the method of BRUCE, ROBBINS and TUFT (1962) and depends upon reaction with acid potassium permanganate and a colorimetric determination of the phosphate as the blue reduction product of the phospho-molybdate. Satisfactory methods for the determination of residues of phosphine or phosphide using gas chromatography have not been published although DUMAS (1964) used gas chromatography with a thermistor detector for gas concentrations in air. Tests are in progress in the Pest Infestation Laboratory using flame ionization and "phosphorus" (caesium bromide) detectors.

(6) *Residues of fumigant mixtures and the development of multidetection procedures*

(a) Work by BIELORAI and ALUMOT (1966) at Rehovot, Israel

These workers determined residues in whole cereals fumigated with a proprietary fumigant containing carbon disulphide, chloroform, carbon tetrachloride and trichloroethylene. They used a distillation-extraction procedure based on KENNET and HUELIN'S (1957) method but with a modified apparatus and with toluene in place of benzene. They obtained good separation of the compounds on a single gas chromatography column and used an electron capture detector.

(b) Work by WIT and GREVENSTUK (1967) at Utrecht

These workers are determining ethylene dibromide (EDB), ethylene dichloride (EDC) and carbon tetrachloride (CTC) in wheat. Extraction is again based on the KENNET and HUELIN method using toluene as solvent, followed by gas chromatography. One column and a flame ionisation detector is used for EDC and a second column and an electron capture detector for EDB and CTC.

- (c) Work by HEUSER and SCUDAMORE at Pest Infestation Laboratory, Slough

Residues of methyl bromide, ethylene oxide, ethylene dibromide and ethylene chlorohydrin have been extracted from flour and from ground and whole wheat with a 5:1 v/v mixture of acetone and water, by shaking in the cold solvent in a stoppered vessel. Aliquots of the clear supernatant liquor were injected into a gas chromatograph using a 15% w/w polypropylene glycol on Chromosorb W column and flame-ionisation detector. A specially designed injection unit was developed for this purpose. Recoveries of these substances were from 95–100%, checked by independent vapour-phase application and subsequent aeration techniques, with chemical analysis of the vapours removed. Carbon disulphide is expected to yield a similar result. It is highly probably that residual amounts of other fumigants such as carbon tetrachloride, ethylene dichloride and acrylonitrile are extracted with equal efficiency by this solvent. However, the proximity of their boiling points to that of acetone makes separation of minute amounts from the solvent peak difficult.

Present investigations are concerned with the use of the electron-capture detector for these and other compounds since it is relatively much less sensitive to acetone, and with the search for a suitably effective higher-boiling solvent which would widen the application of the flame ionisation detector.

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Appendix XVI

Extract from the Joint Report of the FAO Working Party and the WHO Expert Committee on Pesticide Residues 14–21 November 1966 (WHO Technical Report No.370, 1967)

Abridged list of acceptable daily intakes, tolerances, practical residue limits of interest in connexion with residue analysis

ADI	Foods	Recom- mended tol- erance	Practical residue limit (temporary) ppm
mg/kg/day		ppm	ppm

Aldrin /dieldrin	0.0001	all foods	none	milk (whole)	0.003
				meat	0.2*
				vegetables	0.05
Carbaryl	0.02	various	down to 0.0		
DDT	0.01	various	down to 1.0	milk (whole)	0.005
				milk products	0.2*
Diphenyl	0.125	citrus	110		
Ethylene dibromide	1.0 as Br	various	down to 20		
Methyl bromide		various	0.1	meat, pots.	0.05
Heptachlor/HE	0.0005			milk (whole)	0.002
				milk products	0.025*
Maltahion	0.02	various	down to 3.0		
Organomercurials	—		—	0.02–0.05	
Pip. butoxide	0.03	cereals	20		
		others	8		
		(various)			
Pyrethins	0.04	cereals	3		
		others	1		
		(various)			
Phosphine	—	cereals	0.1		
		(raw)			
gamma-BHC	0.0125	various	down to 0.5	milk	0.1*

* On a fat basis

H. EGAN

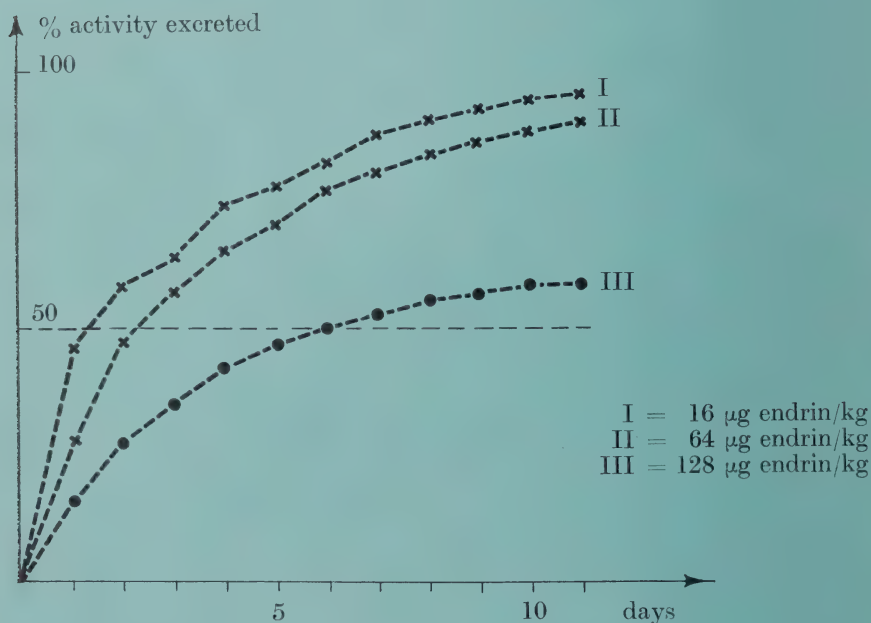


Fig. 1 Excretion of endrin after oral application

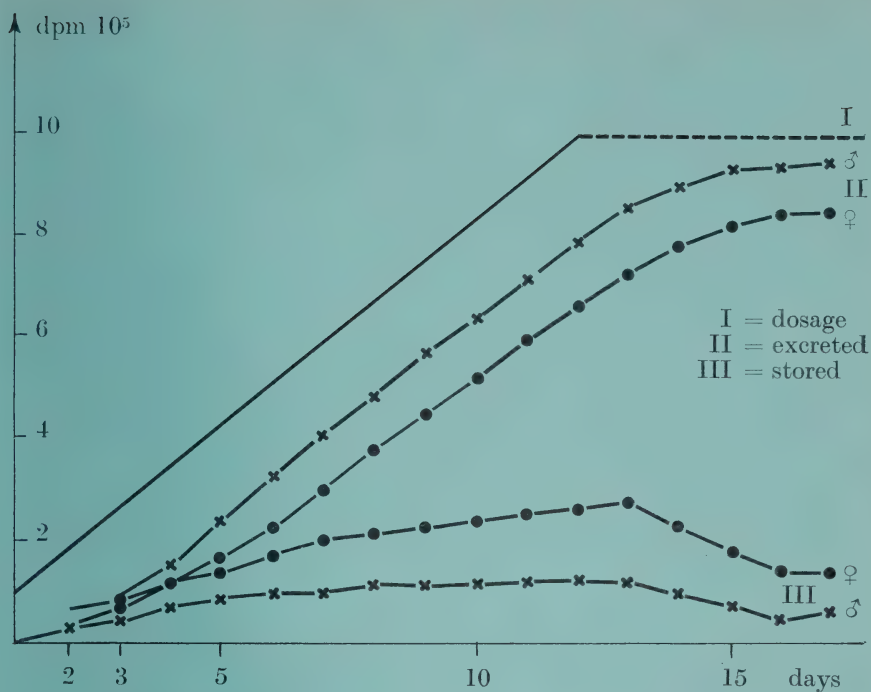


Fig. 2 Storage and excretion of endrin- ^{14}C after oral administration to rats

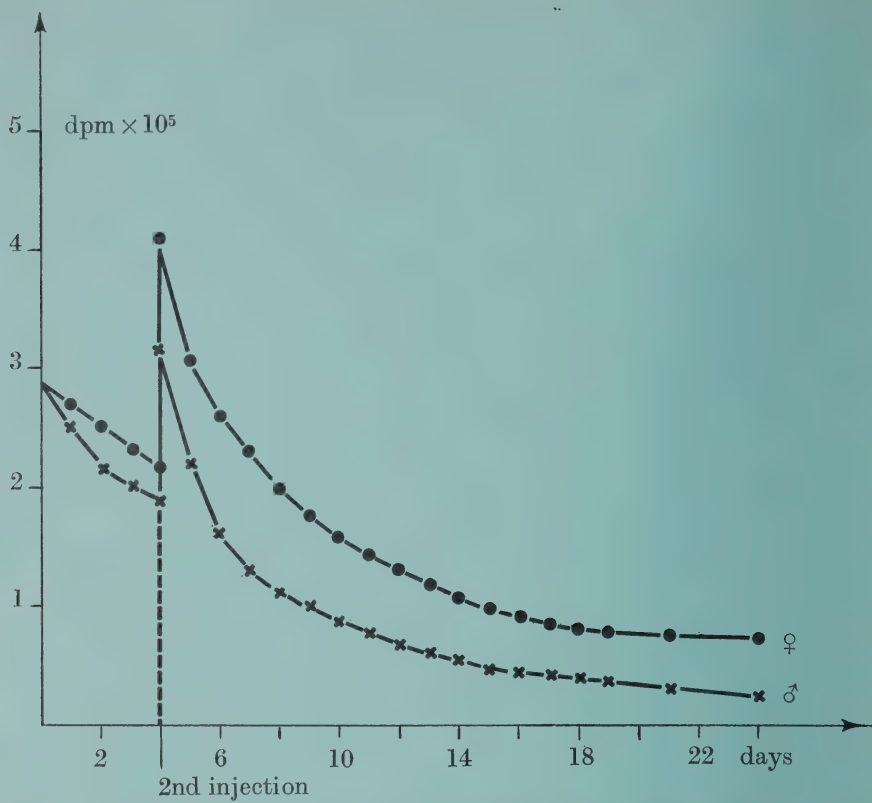


Fig. 3 Radioactivity stored in rats after intravenous injection of 200 $\mu\text{g/kg}$ endrin- ^{14}C

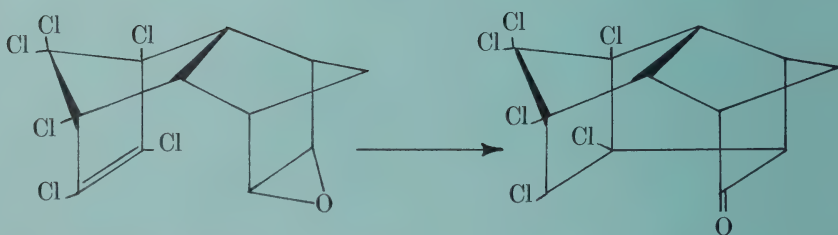


Fig. 4 Keto-rearrangement of aldrin

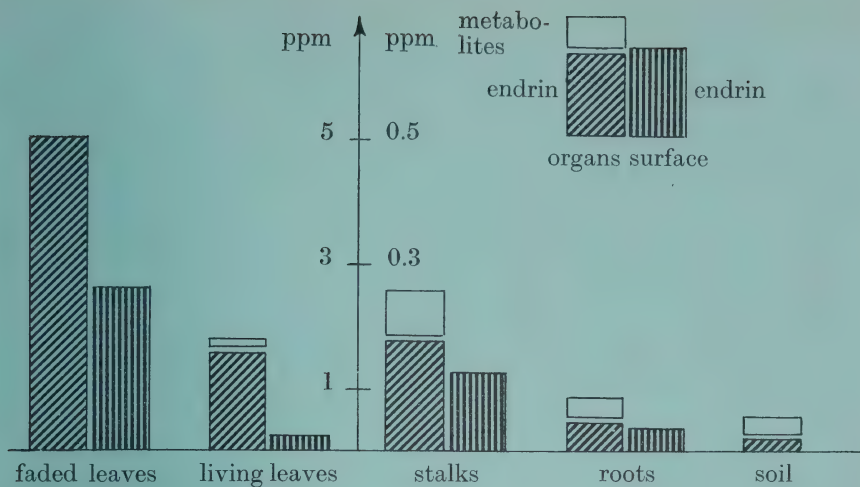


Fig. 5 Endrin concentrations and rates of metabolism in the organs of cabbage

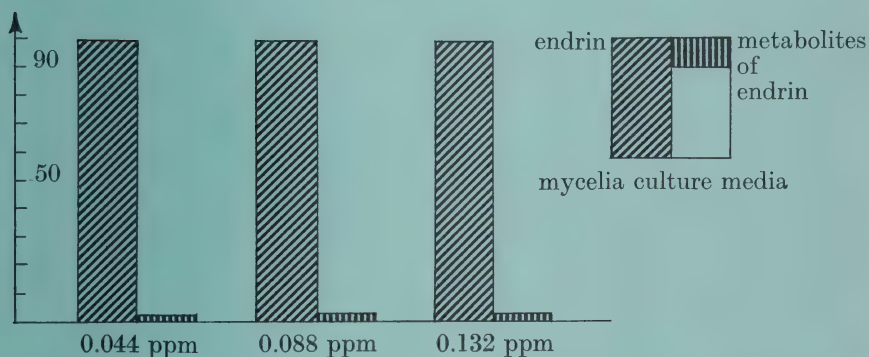


Fig. 6 Distribution of radioactivity in mycelia and culture media *Aspergillus flavus*

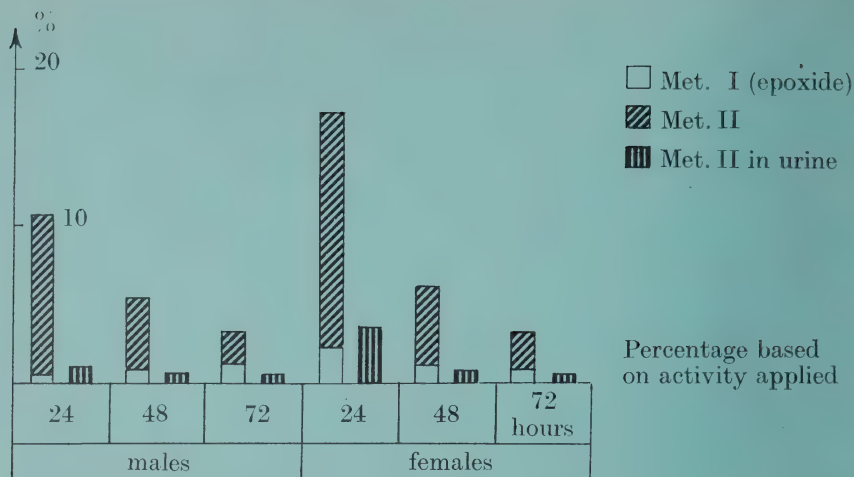
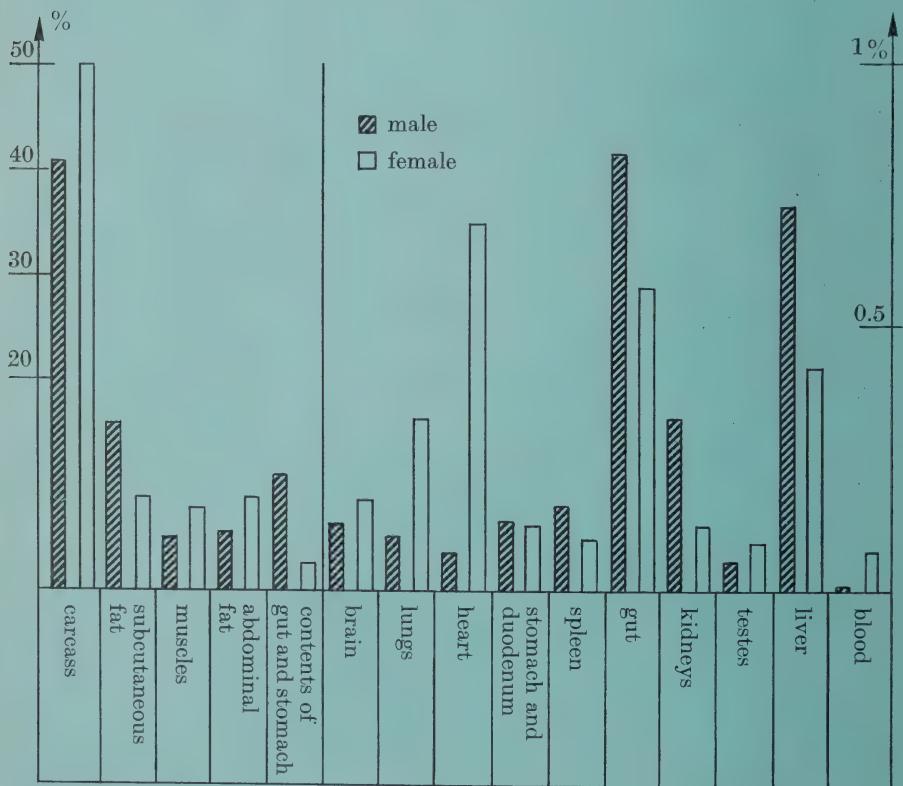


Fig. 7 Excretion and metabolism of heptachlor- ^{14}C by rats after intravenous administration of $25\text{ }\mu\text{g}$ per animal



Percentages based on the recovered amount of radioactivity

Fig. 8 Distribution of radioactivity 72 hours after intravenous administration of $25\text{ }\mu\text{g}$ heptachlor- ^{14}C to rats

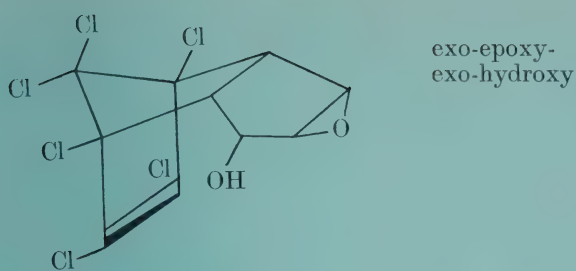


Fig. 9 Hydrolysis product of isobenzan metabolite

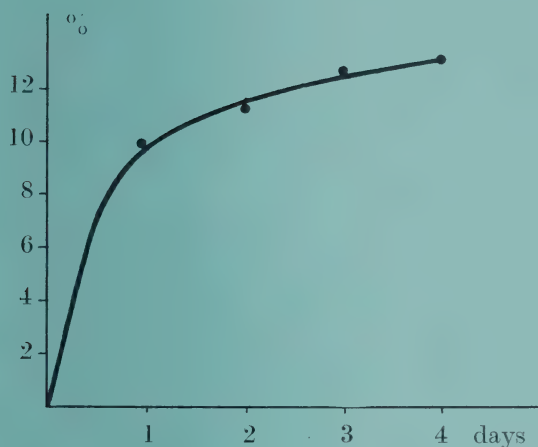
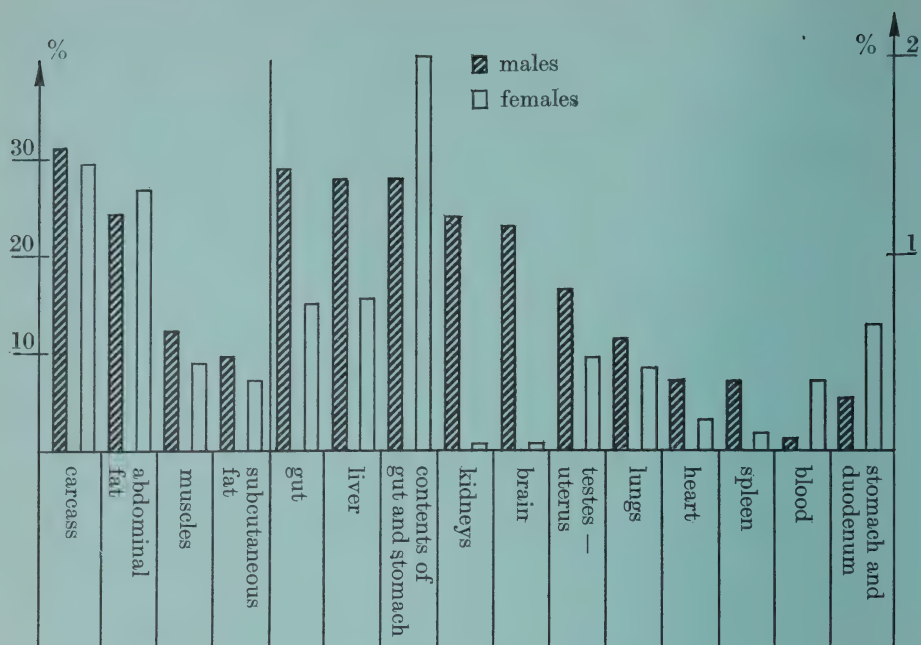
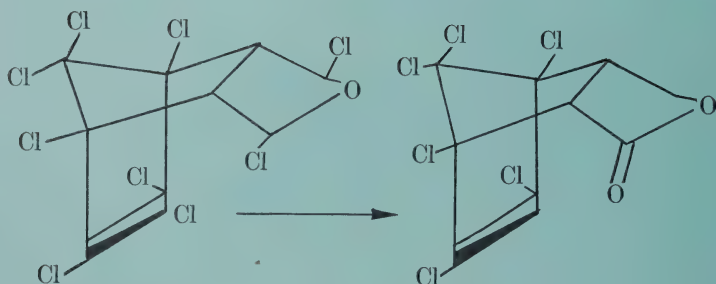


Fig. 10 Excretion of activity after intravenous injection of 241 $\mu\text{g/kg}$ Telo-
drin- ^{14}C in male rabbits



Percentage based on activity applied

Fig. 11 Distribution of radioactivity in rats 48 hours after intravenous administration of 7 µg/animal Telodrin-¹⁴C



Percentages based on activity administered

Fig. 12 Hydrolysis product of isobenzan metabolite

Table I Distribution and concentration of radioactivity in male rats 24 hours after intravenous administration of 40 μ g of endrin- 14 C

	%* activity	ppm**
liver	10.0	0.24
heart	4.1	1.27
kidneys	1.4	0.27
lungs	1.0	0.23
spleen	0.3	0.18
stomach and duodenum	0.7	0.13
gut	1.9	0.08
testes	2.3	0.18
brain	4.0	0.65
abdominal fat	38.2	0.90
subcutaneous fat	4.1	0.12
blood	4.3	0.26
contents of gut and stomach	11.8	0.61
muscles	4.8	0.02
carcass	5.6	0.03
skin	5.4	0.04

* Percentages based on the activity in the bodies without tail where injection was applied

** Concentration based on the molecular weight of endrin

Table II Distribution and concentration of radioactivity in the body of rats after 12 days feeding with endrin- 14 C

	Day 13 (two animals)		Day 17 (four animals)	
	%* activity	ppm**	%* activity	ppm**
liver	5.4	0.28	6.5	0.075
heart	1.3	0.58	0.5	0.080
kidneys	2.0	0.29	1.0	0.068
lungs	4.1	0.30	3.2	0.126
spleen	3.0	3.0	1.2	0.415
stomach and duodenum	2.0	0.67	1.2	0.100
gut contents	14.8	1.03	7.0	0.057
uterus or testes	0.7	0.9	2.6	0.600
brain	1.0	0.25	1.0	0.080
abdominal fat	16.9	0.38	24.4	0.142
skin and subcutaneous fat	33.0	0.74	42.6	0.240
blood	5.7	1.1	1.5	0.034
muscles	8.2	0.06	6.0	0.001
bones	2.4	0.04	2.5	0.001

* Percentages based on the radioactivity present in the bodies

** Concentration in ppm based on the molecular weight of endrin

1968

**October Next Bureau Meeting
29-30**

August 18-25	Joint National Meeting on Clinical Chemistry	Washington* D.C.
August 25-30	VIth International Symposium on Reactivity of Solids	Schenectady (USA)
September 2-6	IIIrd International Symposium on Fermentation	New Brunswick (USA)
September 3-6	International Symposium on Macromolecular Chemistry	Toronto (Canada)
September 4-6	International Conference on Electrophotography	Rochester* (USA)
September 8-12	XIth International Conference on Coordination Chemistry	Haifa (Israel)
September 9-12	Symposium on Valence Tautomerism	Karlsruhe (Germany)
September 10-13	Analytical Chemistry Symposium	Warsaw (Poland)
September 10-13	Chemical Aspects of Paper Making	Prague (Czechoslovakia)
September 16-18	XIth International Conference on Coordination Chemistry	Jerusalem (Israel)
September 16-19	Microsymposium on Structure of Organic Solids in Macromolecular Chemistry	Prague (Czechoslovakia)
September 23-26	Microsymposium on Distribution Analysis and Fractionation of Polymers	Prague (Czechoslovakia)
1968 or later	Carbohydrate Chemistry	Paris (France)
1969		
February 2-9	X Congreso latinoamericano de Química	San José (Costa Rica)
April 21-25	Symposium on Natural Products, in particular Steroids and Terpenes	México City (México)
May 27-30	Société de Chimie Physique	Paris (France)
July 1st decade	XXVth International Conference of Pure and Applied Chemistry	Cortina d'Ampezzo (Italy)
July 14-18	IVth International Congress on Pharmacology	Basle* (Switzerland)
July 14-18	International Conference on Atomic Absorption Spectroscopy	Sheffield (UK)
July 14-20	International Symposium on Chemical Control of Human Environment	Johannesburg (S. Africa)
July 17-19	Symposium on Surface Area Determination	Bristol (UK)
July 21-25	International Symposium on Analytical Chemistry	Birmingham (UK)

July 27– August 1	IVth International Symposium on Organometallic Chemistry	Bristol (UK)
August 20–27	XXIInd International Congress of Pure and Applied Chemistry and XIIth International Conference on Coordination Chemistry	Sydney Australia)
August 25–30	Symposium on Kinetics and Mechanism of Polymerization	Budapest (Hungary)
September 8–13	VIIth International Congress of Clinical Chemistry	Geneva (Switzerland)
September 9–12	International Symposium on Conformational Analysis	Brussels (Belgium)
To be decided 1969 or 1970	Symposium on Nonaqueous Electrochemistry Cyclo-Addition	To be decided * Munich (Germany)
	1970	
Beginning	Analytical Congress	Budapest (Hungary)
July	VIth International Symposium on Chemistry of Natural Products VIth International Symposium on Microchemistry Symposium on Carbohydrate Chemistry (Division of Organic Chemistry) Symposium on Macromolecular Physics (Macromolecular Division)	Riga (USSR) Graz (Austria) Leiden or Delft (Netherlands)
	1971	
July	XXVIth International Conference of Pure and Applied Chemistry XXIIIrd International Congress of Pure and Applied Chemistry Symposium on Macromolecular Chemistry	Washington, DC (USA) Boston (USA) Boston (USA)

LIST OF ABBREVIATIONS

CBN	Commission on Biological Nomenclature
CIG	Comité International de Géophysique
CIOMS	Council for International Organizations of Medical Sciences
COSPAR	Committee on Space Research
ECOSOC	Economic and Social Council of United Nations
FAGS	Federation of Astronomical and Geophysical Services
FAO	Food and Agriculture Organization
IAEA	International Atomic Energy Agency
IAMS	International Association of Microbiological Societies
IASH	International Association of Scientific Hydrology
IAU	International Astronomical Union
IBP	International Biological Programme
IBRO	International Brain Research Organization
ICRO	International Cell Research Organization
ICSU	International Council of Scientific Unions
IGU	International Geographical Union
IGY	International Geophysical Year
IMU	International Mathematical Union
IQSY	International Years of the Quiet Sun
ISO	International Organization for Standardization
ITU	International Telecommunication Union
IUB	International Union of Biochemistry
IUBS	International Union of Biological Sciences
IUCr	International Union of Crystallography
IUCN	International Union for the Conservation of Nature and Natural Resources
IUCRM	Inter-Union Commission on Radio Meteorology
IUGG	International Union of Geodesy and Geophysics
IUGS	International Union of Geological Sciences
IUNS	International Union of Nutritional Sciences
IUPAC	International Union of Pure and Applied Chemistry
IUPAP	International Union of Pure and Applied Physics
IUPS	International Union of Physiological Sciences
IUTAM	International Union of Theoretical and Applied Mechanics
JCAM	Joint Commission on Atomic Masses
JCAR	Joint Commission on Applied Radioactivity
SCAR	Scientific Committee on Antarctic Research
SCOR	Scientific Committee on Oceanic Research
UMC	Upper Mantle Committee
UNESCO	United Nations Educational, Scientific and Cultural Organization
URSI	Union Radio Scientifique Internationale
WDC	World Data Centre
WHO	World Health Organization
WMO	World Meteorological Organization

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**INTERNATIONAL UNION OF PURE
AND APPLIED CHEMISTRY**

**UNION INTERNATIONALE DE CHIMIE
PURE ET APPLIQUÉE**

50 YEARS IUPAC


1918–1968

**INFORMATION BULLETIN
NUMBER 33**

DECEMBER 1968

SECRETARY GENERAL:

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PREFACE

The US National Academy of Sciences appointed a Committee under the chairmanship of Prof. W.A. NOYES, our distinguished former Past President, to study, for internal use in the United States exclusively, "The Quality and Organization of International Scientific Meetings". This report is addressed directly to the Foreign Secretary of the US National Academy of Sciences. The content of the report however, is a most valuable document, also for the International Union of Pure and Applied Chemistry and gives excellent information for all organizing committees within IUPAC. I therefore have asked Prof. NOYES and the Foreign Secretary of the National Academy of Sciences for the permission to publish the first 5 pages of this report. This permission was granted by letter and thanks are expressed herewith to the US National Academy of Sciences.

Dr RUDOLF MORF, Secretary General

REPORT OF THE COMMITTEE ON THE QUALITY AND ORGANIZATION OF INTERNATIONAL SCIENTIFIC MEETINGS

TO THE FOREIGN SECRETARY OF THE NATIONAL ACADEMY OF SCIENCES

Introduction

The National Academy of Sciences formed this Committee to study the quality and organization of international scientific meetings because of the feeling that although such meetings are undeniably useful and necessary, their quality is uneven and many could be better than they are. An effort has been made to identify strong and weak points of meetings as they are now being held and to recommend measures for their improvement.

The study has been limited to meetings held under international auspices and, more especially, to meetings of international organizations of which the Academy is a member. Some recommendations may also be applicable to other types of meetings.

We are grateful to Dr WILLIAM D. GARVEY, Center for Research in Scientific Communication, Johns Hopkins University, and to Mrs HELENA B. LEMP, Congress Manager, Federation of American Societies for Experimental Biology, for expert advice and many helpful suggestions.

Objectives of international scientific meetings

To place our findings in proper perspective, it is useful to state briefly the main objectives served by international scientific meetings:

- (1) Exchange of scientific information:
 - (a) about completed research. Reports are integral parts of meetings, but meetings also give participants the opportunity for informal discussions with each other
 - (b) about research in progress
 - (c) about plans for future research
 - (d) about research techniques not described in published reports

- (2) Formulation of agreements on symbols, units, and nomenclature
- (3) To provide the organizational framework necessary for international scientific cooperation
- (4) To establish personal contacts among scientists:
 - (a) as a basis for the subsequent exchange of information and materials by mail and possibly for the exchange of personnel
 - (b) for identifying the most active foreign scientists in one's field
 - (c) for comparing the approach and quality of one's own research with that of scientists in other institutions and countries
- (5) To reduce the technological gap by making research in the scientifically advanced countries known throughout the international scientific community

An additional objective of international scientific meetings would be to improve scientific communication and cooperation among scientists and technologists in developing countries, as well as between similar persons in industrial and pre-industrial countries. Most scientific and technical meetings are held in highly industrialized countries, but it would be desirable to hold more meetings in developing regions. These might deal with problems of interest to the geographical regions in question. Various groups have taken an interest in this problem, for example: in the Academy, the Science Organization Development Board and the US National Committee for the International Biological Program (IBP); in the International Council of Scientific Unions, the Committee on Science and Technology in Developing Countries and the Special Committee for the IBP; and in Unesco, both Departments of Science. The total effort is still small and much more should be done.

Factors affecting the quality of international scientific meetings

Three important factors determine the quality of a meeting: scientific program, invited speakers, and the chairmen of sections. Important as these matters are, they are now sometimes left to the discretion of national organization in our opinion often fails to meet its prime responsibility to ensure quality. We recommend, therefore, that international organizations which sponsor meetings take more active parts in planning. For financial reasons, it may not always be possible for the international sponsor to be represented at meetings of the national organizing committee, but before planning begins, it can set the main lines of the program, and later it can monitor the development of the program and can recommend changes and improvements, as may be necessary.

- (1) The quality of papers presented determines to a large degree the character of a meeting. We therefore recommend that international sponsors of meetings assume responsibility for ensuring that screening of contributed papers is carefully and rigorously done. The mechanism for this is best left to the discretion of the international sponsor rather than to a single country. The presentation of fresh material must be encouraged. The time limit for the various stages of screening must be established so that the deadline for the submission of reports is as late as possible. — The Academy should let it be known that whenever it considers screening to be adequate, it can more strongly recommend the use of public funds to facilitate American participation.

- (2) There is almost universal agreement among scientists that informal discussions are one of the most useful, if not the most useful, means of exchanging ideas and information. It is of great importance to make sure that physical arrangements are conducive to informal contacts. In the immediate vicinity of the meeting rooms there should be lounges or coffee rooms where participants can get together easily and comfortably for conversation. Moreover, the program should not be so tightly scheduled as to preclude organization of impromptu meetings of scientists who find they have some common interest to discuss. A free afternoon for an excursion or an unencumbered evening often provides this occasion.
- (3) Good physical facilities are indispensable to the success of meetings. If meeting rooms are small or improperly designed, if meeting-room equipment such as the public address system, the projector or the screen are inadequate, or if the projectionist, the interpreter or other meeting-room personnel are insufficiently trained, meetings will suffer no matter how good the scientific program. The need for attention to physical arrangements is, of course, not confined to the meeting room. There are the questions of housing, of meal service—particularly between morning and afternoon sessions, of communications between organizers and participants, of transportation housing and meeting areas, to mention but a few matters that often require attention. One particularly frequent cause of complaint at big meetings is the difficulty of locating colleagues. Therefore, it is probably worth while to make special mention of the importance of a message center and directory service and the desirability of badges with name and specialty in large capital letters for easy reading.

Since the success of a meeting may well rest on the adequacy of physical facilities, organizers are urged to give careful attention to this aspect of preparations. The task of organizers will be easier if they can draw upon the experiences of persons within the international organization which is sponsoring the meeting. This is particularly true in the case of large meetings because few scientists have the experience of organizing more than one large meeting in their lifetimes. Consequently, the members of national committees organizing large meetings generally lack previous experience. International organizations may therefore find it in their interest to set up an international committee of key organizers of the past to whom the present national organizing committee can turn for advice.

Since we have found poor physical arrangements to be the main problem encountered at large scientific meetings, we shall return to this subject in the next section of this report.

Large and small international scientific meetings

The Committee considers that it would serve little purpose to endorse one of these two kinds of meetings in preference to the other. It would be more useful, in our opinion, to discuss the advantages and problems of each.

(1) *Large meetings*

There are several advantages peculiar to large meetings:

- At large meetings, there is often greater opportunity for interdisciplinary confrontation. The scientist who takes part in a large

meeting where many different specialties are represented not only has the opportunity to take a broad look at his field, but he often has the stimulating experience of meeting colleagues outside his specialty who approach problems from an entirely different point of view.

- At large meetings there is incontestably the opportunity for a large number of scientists to listen and to be heard. This is important for young scientists who are rarely invited to small meetings where the number of participants is restricted.
- Large meetings are probably more economical on a *per capita* basis. One meeting of 5000 participants costs less than, say, 25 meetings of 200 persons each.

The overriding problem of large meetings is the need of proper organization. The difference between large and small meetings is not one of degree but of kind. Consequently, two distinct techniques of organization are involved. Perhaps the biggest difference is in the relative need for a secretariat. For a small meeting the services of an efficient and experienced secretariat may not be necessary, but in the case of a large one such services are indispensable. Therefore, we recommend that the budget of every large meeting include funds for a secretariat which can attend to the myriad details of organizing and running such a meeting. In the case of the largest meetings, it is usually desirable to have the services of a professional congress organizer, but persons properly qualified for this position are not easy to find. On the other hand, there are generally available handbooks for the guidance of those organizing meetings. Two examples are *The Planning of International Meetings*, issued by the Council for International Organizations of Medical Sciences, and *Congress Organizers' Manual*, published by the Union of International Associations. Mrs. LEMP, who is mentioned in the introduction, has also prepared a handbook on the organization of international scientific meetings which she expects to publish in 1968. Perhaps the most important element of such handbooks is the timetable, describing at what point various actions should be taken in preparation for the meeting.

Another good source of advice is one mentioned above, namely, past organizers of meetings. As already suggested, international unions may wish to consider establishing committees of past organizers to advise those who currently have this task.

The Committee believes that the availability of facilities places an upper limit of about 5000 or 6000 participants on large international scientific meetings. There are few cities that can accommodate such a large number of people. Therefore, recurring congresses meeting in a variety of locations generally must limit themselves to a substantially lower figure. The size of a meeting may be limited by restricting the scope of the program, the number of registrants, or the number of papers which can be presented, or by employing a combination of these restrictions.

The Committee believes that one advantage of large meetings—namely, the opportunity to hear papers in fields different from, but related to, one's own—is lost if the meeting is divided into sections which are dispersed in various districts of the same city or scattered widely geographically. Because of the difficulty participants find in getting back and forth between different sessions, the net effect is that of holding several smaller meetings. Therefore, we recommend that the meeting rooms for the various sessions of a large meeting be kept as close together as possible.

(2) *Small meetings*

The quality and organization of small international scientific meetings do not pose major problems.

On the other hand, there appear to be too many small meetings. This tendency could probably be checked if international organizations were to impose realistic limitations on the number of meetings sponsored in a given year, and if they backed up sponsorship with some financial support. This last point is particularly important. If an organization, in agreeing to sponsor a meeting, not only granted permission to use its name in connection with the meeting but committed itself to financial support, the desirability of conferring sponsorship would no doubt be much more carefully considered than may be the case at present. We recommend, therefore, that each international scientific union determine for itself what constitutes a reasonable number of meetings to be held in its discipline in one year; that it then adopt the policy of limiting its sponsorship to that number; and that it accompany sponsorship with some degree of financial support. This policy would tend not only to keep the number of meetings down but to improve the quality of those that are held. In granting sponsorship, the union should satisfy itself (1) that there is a real need for the meeting; (2) that the meeting promises to be of high quality; and (3) that it does not unnecessarily duplicate any other meeting. At home, granting agencies could reinforce this policy by showing preference, in the award of travel grants, for meetings sponsored by unions with such a policy.

Two ways may be suggested to avoid unnecessary duplication of meetings:

- Establishment of permanent channels of communication among unions to deal with this problem. An outstanding example of such a mechanism now in existence is the Inter-Union Commission on Solar Terrestrial Physics, which has this and other co-ordination functions. Another example is that of the representatives of the biological unions in the International Council of Scientific Unions (ICSU) who met before the meeting of the ICSU Executive Committee last October, mainly to coordinate meetings. The next time, representatives of non-ICSU unions may be invited to attend in the interest of broader coordination. We applaud this initiative, and we hope that other disciplinary groupings of unions will follow suit.
- Another way of reducing duplication is through better use of periodically published lists of forthcoming international scientific meetings. Several such lists are the *International Congress Calendar* of the Union of International Associations, the list of forthcoming meetings in the *ICSU Bulletin*, the *World List of Future International Meetings* issued by the Library of Congress and *World Meetings outside USA and Canada* published by Technical Meetings Information Service. There are others, some of which are put out by national scientific agencies of various countries. We recommend that organizers of prospective meetings, in the early stages of planning, consult such lists to determine whether their meeting would duplicate another in a more advanced state of planning, or whether it could be combined to advantage with another on a related topic. Organizers should also assume the responsibility of seeing that meeting are brought to the attention of as many potential participants as possible by means of notices in these lists.

The financing of international scientific meetings

International scientific organizations will find it easier to exert a beneficial influence on the planning of meetings if at the same time they assume greater responsibility for financing them. Financial assistance to organizers would probably be most valuable in the early stages of planning, before there are any receipts from the registration fee. We recommend that each Union consider the establishment of a revolving fund from which organizers can obtain loans of \$5,000 to \$10,000. The International Union of Biological Sciences and the International Union of Physiological Sciences already are doing this. There are various ways in which money could be raised for such funds. The following are two possibilities: (1) The Union might appoint an international fund-raising committee which could make use of the personal contacts of the members to seek contributions from various sources, including industrial firms and foundations. (2) Place a surcharge of, say, \$2 on the registration fee of each Union-sponsored meeting to provide seed money for the next meeting in that particular series.

The International Council of Scientific Unions may also wish to consider the desirability of making loans to Unions for the organization of meetings from its Working Capital Fund.

The publication of papers presented at international scientific meetings

Caution must be exercised in making any general recommendation on this point because we find there are wide differences of practice and opinion not only from field to field but also within fields. Therefore, the only advice we are inclined to give is this: *the publication of proceedings should not be undertaken automatically*. The desirability of all possible forms of publication should be studied, and if the choice is proceedings, this should be the result of a real need.

Addendum

If it may be permitted, the Secretary General would like to make an additional remark to this excellent report:

Learned societies, universities, national academies, governmental and non-governmental research institutes should be urged to delegate young chemists to attend congresses and symposia with the task to listen, to study, and to learn how scientific information and communication is best achieved.

The old-fashioned way of appointing delegates to congresses, symposia, etc., granting reimbursement for travel and living costs only if they read a paper, should be abolished completely.

As a result of this change, as suggested above, the quality of congresses and symposia will increase.

**XXIIND INTERNATIONAL CONGRESS OF PURE
AND APPLIED CHEMISTRY**
AND
**XIITH INTERNATIONAL CONFERENCE
ON COORDINATION CHEMISTRY**

These two events will be the highlight of IUPAC's activity in 1969. All details with respect to the International Congress and the Conference on Coordination Chemistry, to take place in Sydney (Australia), are fixed and the programme has been distributed as well as published in Information Bulletin No. 32 (pages 5, 6, 7).

**XXVTH International Conference
of Pure and Applied Chemistry**

will be held at the invitation of Consiglio nazionale delle Ricerche, Roma, at
Cortina d'Ampezzo.

The tentative programme is:

Friday, 4 July: All day meeting of the Bureau
Saturday, 5 July: Full day, 1st Council meeting
Monday, 7 July: 2nd Council Meeting (elections)
Tuesday, 8 July: XXIVth Meeting of the new Bureau

The meetings of the Divisions, Sections, and Commissions will be organized in detail, according to the wishes expressed by the respective Presidents. The detailed programme will be published in the Information Bulletin No. 34, early next year.

Cortina d'Ampezzo is a world famous centre for winter sports. The XXVth IUPAC Conference is scheduled in such a way that there is no conflict with the very busy summer season. The average temperature is about 25 °C in the daytime and falls to about 10 °C–15 °C at night. Although the weather is usually excellent, it is advisable to bring rain wear. The dress throughout the Conference shall be informal.

The nearest airports are la Venezia (Venice), 155 kilometers, and Milano, 450 kilometers. An excellent opportunity for travelling to Cortina d'Ampezzo is provided from the Zürich airport by comfortable bus, which travels over the highest European pass, Stelvio, 2700 meters (8000 ft) through the most beautiful alpine scenery.

DETAILED INFORMATION REGARDING FORTHCOMING EVENTS

INTERNATIONAL SYMPOSIUM ON NATURAL PRODUCTS SYMPOSIUM INTERNACIONAL DE PRODUCTOS NATURALES

Mexico City, 21-25 April 1969

The International Union of Pure and Applied Chemistry (IUPAC) and the Mexican Chemical Society (SQM), are pleased to invite you to the International Symposium on Natural Products which will be held in Mexico City, Mexico from 21 to 25 April 1969.

This Symposium will deal especially with steroids and terpenes and will take place according to the rules and program described below.

Submission of Papers

Original contributions related to the topics of the Symposium are invited. The presentations should be 15 to 20 minutes long, and a selection of the papers submitted will be made by the referees. Closing date for submission of papers is 1 November 1968. An abstract of no more than 1000 words must accompany the paper submitted.

Plenary Lectures

The titles and authors of the Symposium lectures are as follows:

- D. H. R. BARTON, Imperial College of Science and Technology, London (UK): Recent advances in steroid chemistry
C. DJERASSI, Stanford University, California (USA): Applications of mass spectrometry in the steroid field
T. A. GEISSMAN, University of California, Los Angeles, Cal. (USA): Studies on lactones of compositae
R. DE GHENGI, Ayerst Laboratories, Montreal (Canada): Synthetic cardenolides and related products
O. JEGER, Eidg. Technische Hochschule, Zurich (Switzerland): Some novel transformations of steroids
S. MORRIS KUPCHAN, University of Wisconsin, Madison (USA): Recent advances in the chemistry of terpenoid tumor inhibitors
J. ROMO, Instituto de Química, Universidad nacional autónoma de México (México, DF): Estudios recientes sobre sesquiterpenos
K. SCHREIBER, Institute for Plant Biochemistry, Berlin (Germany): Recent advances in the chemistry of plant steroids
F. ŠORM, Czechoslovak Academy of Science, Praha 6 (CSR): Recent advances in terpene chemistry
K. TAKEDA, Shionogi Research Laboratories, Osaka (Japan): Sesquiterpenes containing an ether-linkage in the molecule

Information

All correspondence should be directed to "IUPAC-SQM Symposium" Sociedad química de México, Apartado postal 4-875. México 4 (DF México)

Official Languages

The official languages will be Spanish and English. There will be no simultaneous translation, but interpreters will be available to translate discussions from Spanish to English.

Publication

Abstracts of papers to be presented at the Symposium will be distributed in advance to all registrants.

XXVTH INTERNATIONAL CONFERENCE ON PURE AND APPLIED CHEMISTRY

Cortina d'Ampezzo, 4—8 July 1969

IVTH INTERNATIONAL CONFERENCE ON ORGANOMETALLIC CHEMISTRY

Bristol, 27 July—1 August 1969

The Fourth International Conference on Organometallic Chemistry will be held in Bristol (UK), from 27 July to 1 August 1969, under the sponsorship of the Chemical Society of London, and the International Union of Pure and Applied Chemistry.

The Conference will be held at the School of Chemistry of the University of Bristol, and accommodation will be available in University Residence Halls. Accommodation for families will be available by private arrangement with local hotels.

A number of symposia will be held within the framework of the conference to allow more detailed discussion of certain topics. Suggestions for symposia topics will be welcome and may be given on the Preliminary Registration Form.

The number of papers to be presented at the Conference will probably have to be limited, and after Abstracts (due 1 March 1969, submitted in English) have been considered, invitations to present papers at the Conference will be issued. Authors may present papers in any language, but since simultaneous translation will not be available it would be preferred if English were used.

Address replies to the Secretary: Dr E. W. ABEL, School of Chemistry, University of Bristol, Cantock's Close, Bristol 8 (UK).

XXIIND INTERNATIONAL CONGRESS OF PURE AND APPLIED CHEMISTRY and

XIITH INTERNATIONAL CONFERENCE ON COORDINATION CHEMISTRY

Sydney, 20—27 August 1969

The Australian Academy of Science extends an invitation to a combined meeting, comprising the XXIInd International Congress of Pure and Applied Chemistry, and concurrently the XIIth International Conference on Coordination Chemistry, which will be held in Sydney, Australia, 20—27 August, 1969.

Scientific Programme

XXIIND IUPAC Congress

The scientific programme will represent the interests of three Divisions of the International Union of Pure and Applied Chemistry—Physical Chemistry, Inorganic Chemistry, and Macromolecular Sciences, and will be presented under the following headings:

Physical Chemistry

1. Theoretical chemistry, and atomic and molecular spectroscopy (incorporating the Seventh Australian Spectroscopy Conference)
2. Intermolecular forces: solids, liquids, gases and solutions, *including a session on*
 - (a) Electrolytes and ionic melts
3. High pressure chemistry
4. Kinetics, *comprising*
 - (a) Reactions of free radicals and excited species
 - (b) Thermally-induced gas-phase reactions
 - (c) Kinetics at the solid/gas interface
 - (d) Rates and equilibria in solutions
5. The solid/liquid interface, *including sessions on*
 - (a) Electrode processes and the double layer
 - (b) Oxide-solution interfaces
6. *Symposium: 50 Years of Valence Theory* (invited speakers only)

Macromolecular Chemistry

1. Polymerization kinetics and the physical properties of polymers, *including sessions on*
 - (a) Graft polymerization
 - (b) Polyelectrolytes

Inorganic Chemistry

1. General inorganic chemistry, *comprising*
 - (a) Non-metals
 - (b) Non-transition metals
2. Mineral chemistry, *comprising*
 - (a) Interfacial processes in mineral extraction
 - (b) On-stream analysis in the mineral industry
3. Solid-state chemistry, *comprising*
 - (a) Preparation and growth of crystals, including vapour transport and hydrothermal synthesis
 - (b) Characterization, including defect solids and non-stoichiometric phases

XIITH International Conference on Coordination Chemistry

Papers will be presented under the following headings:

1. The nature of the metal-ligand bond in coordination complexes
2. Biological aspects of coordination chemistry
3. Mechanisms of substitution and electron-transfer reactions
4. Investigation of molecular dissymmetry
5. Complex equilibria in solution
6. Reactivity of coordinated ligands and catalysis by coordination compounds
7. Structure and reactivity of organometallic compounds

All scientific proceedings will take place in a compactly-sited group of lecture theatres in the University of Sydney. While the IUPAC and ICCC meetings will run concurrently, participants will be able to move freely from one to the other if they so wish.

In either programme the committee may accept papers of exceptional interest on topics other than those listed.

Plenary Lectures

The following have already accepted invitations to deliver plenary lectures: C.A.COULSON (UK), R.DAUDEL (France), B.V.DERJAGUIN (USSR), E.O.FISCHER (Germany), O.FOSS (Norway), E.U.FRANCK (Germany), D.H.FÜRSTENAU (USA), P.HAGENMULLER (France), J.O.HIRSCHFELDER (USA), J.JORTNER (Israel), B.B.MALMSTRÖM (Sweden), S.F.MASON (UK), R.S.MULLIKEN (USA), I.E.NEWNHAM (Australia), S.OKAMURA (Japan), C.SCHÄFFER (Denmark), H.TAUBE (USA), and G.WILKINSON (UK).

At least thirty invited Section Lectures will also be given.

Scientific Contributions

Those wishing to contribute papers are requested to indicate this on the preliminary application form. A title and abstract will be required when the final application form is returned; further details will appear in the second circular.

Registration

If you wish to attend you should complete the preliminary application form and mail it without delay. This will not commit you to attending, but return of the completed form will ensure that you receive further information and will greatly help the organizers. The second circular will be distributed later in 1968 to all those who have returned the preliminary application form. The registration fee will be \$27 (Australian currency) or US\$30 for active participants, and \$10 (Aust.) or US\$11 for students and accompanying members.

Correspondence

All correspondence concerning the meeting should be addressed to:

The Chairman, Organizing Committee, XXII IUPAC/XII ICCG
Box 2249U, G.P.O., Melbourne (Australia 3001)
Telex: 30236, Cables and Telegrams: Coresearch, Melbourne

Associated Meeting

An International Symposium on Electron and Nuclear Magnetic Resonance will be held at Monash University, Clayton, Victoria, under the auspices of the Australian Academy of Science, 11-14 August 1969.

Further information concerning this Symposium can be obtained from The Executive Secretary, Australian Academy of Science, Gordon Street, Canberra City, A.C.T. (Australia 2601).

INTERNATIONAL SYMPOSIUM ON CONFORMATIONAL ANALYSIS

Brussels, 9-12 September 1969

List of lecturers of plenary lectures:

Prof. J. DALE, Oslo (Norway)
Prof. J. DUNITZ, Zürich (Switzerland)
Prof. E. L. ELIEL, Notre-Dame (USA)
Prof. R. U. LEMIEUX, Edmonton, Alberta (Canada)
Prof. K. MISLOW, Princeton (USA)
Prof. L. J. OOSTERHOFF, Leiden (Netherlands)
Dr J. OTH, Union Carbide, Brussels (Belgium)
Prof. A. RASSAT, Grenoble (France)
Prof. M. J. T. ROBINSON, Oxford (UK)
Prof. J. SICHER, Prague (Czechoslovakia)

SYMPOSIUM ON THE CHEMISTRY OF NATURAL PRODUCTS

Riga, June 1970

The Symposium sponsored by the IUPAC will be held in Riga in the last decade of June 1970. The organization of the Symposium has been undertaken by the USSR Academy of Sciences which has appointed for this purpose an Executive Committee (Chairman: Prof. YU. A. OVCHINNIKOV) and Scientific Programme Committee (Chairman: Prof. A. S. KHOKHLOV). The Honorary President of the Symposium will be Prof. M. M. SHEMYAKIN.

The Symposium will be devoted mainly to the chemistry of biologically active biopolymers and bio-regulators. Within the programme of the Symposium it is planned to hold 12 plenary lectures, including one dealing with a survey of recent Soviet work and to organize separate sections on the following topics:

- A. Chemistry of peptides and proteins
- B. Chemistry of nucleic acids and nucleotides
- C. Chemistry of lipids including the physical chemistry of membranes
- D. Chemistry of carbohydrates

- E. Chemistry of other natural products (steroids, antibiotics, alkaloids, terpenes, etc.)
- F. Physical methods

It is hoped that the following eminent scientists to whom invitations have been sent will give plenary lectures:

Prof. D. H. R. BARTON (UK), Prof. C. DJERASSI (USA), Prof. H. B. KHORANA (USA), Prof. D. E. KOSHLAND (USA), Prof. E. LEDERER (France), Prof. K. NAKANISHI (Japan), Prof. V. PRELOG (Switzerland), Prof. M. M. SHEMYAKIN (USSR), Prof. F. ŠORM (Czechoslovakia), Prof. F. B. STRAUB (Hungary), Prof. L. L. M. VAN DEENEN (Netherlands), and Prof. R. B. WOODWARD (USA).

It is also proposed to hold 3 Presymposium meetings especially devoted to the chemical aspects of (1) enzyme action, (2) biological membranes and (3) antibiotics.

The first circular containing information on the organizational matters of the Symposium will be issued this autumn.

All inquiries concerning the Symposium should be addressed to the General Secretary of Organizing Committee of the Symposium whose headquarters are in the Institute for Chemistry of Natural Products, Ul. Vavilova 32, Moscow, USSR.

UK CONSORTIUM ON CHEMICAL INFORMATION

The formation of a UK Consortium on Chemical Information is announced.

In August 1966 The Chemical Society established, at Nottingham University, The Chemical Society Research Unit in Information Dissemination and Retrieval. The intention was to create, on behalf of the whole chemical community, an understanding of the needs and problems involved in the establishment of nationally organized chemical information services in this country and to ensure that the necessary knowledge and expertise were acquired to permit the introduction and operation of such services.

The activities which appeared to show most promise of leading to comprehensive mechanized information services in chemistry in the foreseeable future were the computer-based research and development operations of the Chemical Abstracts Service of the American Chemical Society, and it was decided that the initial work at Nottingham should be on user studies of some of the CAS experimental computer-based services.

The Office for Scientific and Technical Information gave financial support to these researches from the early days and such Government support now represents a very substantial part of the budget of The Chemical Society Unit at Nottingham, the Society itself providing the remainder.

Because of the then lack of expert knowledge and trained personnel in the UK the early work was necessarily on a limited scale, but an understanding of and ability to undertake research on the problems involved has now been achieved. It had always been the intention, when this situation was reached, to broaden the basis of study and operation by inviting the collaboration of all organizations whose members require chemical information.

At a meeting called by OSTI in February to consider the UK reaction to proposals being made in OECD there was strong support for the view that there should be greater inter-Society collaboration on matters in the chemical information field, and The Chemical Society was invited to sponsor the creation of a suitable organization.

The resulting Consortium on Chemical Information initially consists of The Chemical Society, The Royal Society, The Royal Institute of Chemistry,

The Society of Chemical Industry, The Faraday Society, The Society for Analytical Chemistry, The Biochemical Society, The Institution of Chemical Engineers, The Chemical Industries Association, and Aslib. OSTI has agreed to be represented by an observer; the Chairman is Dr J.W. BARRETT and the Secretary Dr L.C. CROSS of The Chemical Society.—The general objectives of the consortium are:

- To ensure the planning, development and ultimate provision of a comprehensive information system in pure and applied chemistry, designed to serve chemists and all other users of chemical knowledge
- to ensure full collaboration with all developments in information services in other sciences and technologies and with chemical services in other countries
- to ensure effective collaboration with and advice to Government departments on chemical information matters on behalf of all chemists and users of chemical knowledge
- to encourage the more effective use of existing and new services, particularly those based on mechanized techniques
- to encourage the improvement of existing services, particularly primary and tertiary publications
- to ensure that the scientific public is alerted to the potentiality of these services and trained in their proper use.

Further information may be obtained from Dr L. C. CROSS, 01-734 9971.
5 September 1968

20^e RÉUNION DE LA SOCIÉTÉ DE CHIMIE PHYSIQUE

Paris, 27–30 mai 1969

La Société de Chimie physique consacrera sa vingtième réunion annuelle à une discussion sur le sujet suivant:

Transitions non radiatives dans les molécules.

Pour tous renseignements s'adresser au Secrétaire général de la Société de Chimie physique, 10, rue Vauquelin, F-75 Paris 5^e (France).

INTERNATIONAL ATOMIC ABSORPTION SPECTROSCOPY CONFERENCE

Sheffield, 14–18 July 1969
(Preliminary Notice)

This Conference is organized by the Atomic Absorption Spectroscopy Group of the Society for Analytical Chemistry and the Spectroscopy Group of the Institute of Physics.

Scope: The Conference will cover all aspects of atomic absorption and atomic fluorescence spectroscopy. Papers will include the following topics:

- Fundamental and theoretical studies
- instrumental developments including automation, methods of atomisation, light sources and spectrometric equipment
- new methods and practical analytical applications

Enquiries: All correspondence and enquiries should be addressed to: AAS Conference Secretary, Society for Analytical Chemistry, 9–10, Savile Row, London W1 (UK).

INTERNATIONAL SYMPOSIUM ON NUCLEAR MAGNETIC RESONANCE SPECTROSCOPY

Birmingham, 15–19 July 1969

This Meeting will be arranged by the Chemical Society, Nuclear Magnetic Resonance Discussion Group.

Main speakers will include: P. DIEHL (Basel), D. F. EVANS (London), L. M. JACKMAN (Pennsylvania), M. KARPLUS (Harvard), K. A. McLAUCHLAN (Oxford).

ACTIVITIES OF THE HUNGARIAN CHEMICAL SOCIETY

In 1969 the Hungarian Chemical Society will organize the following meetings:

- *Symposium on Metal Working Oils* at Esztergom (Hungary), 28–30 May 1969. Address: Hungarian Chemical Society, Budapest, V., Szabadság tér 17
- *Symposium on Gas Kinetics* at Szeged (Hungary), 9–12 July 1969. Address: Dr T. BÉRCES, Secretary of the Symposium on Gas Kinetics, c/o Institute of General and Physical Chemistry, The University of Szeged, Szeged, PO Box 105 (Hungary)
- *2nd Hungarian Conference on Ion Exchange* at Balatonszéplak (Hungary), 10–14 September 1969. Address: Hungarian Chemical Society, Budapest, V., Szabadság tér 17

NATIONAL CONGRESS (50TH ANNIVERSARY) OF THE POLISH CHEMICAL SOCIETY

Cracow (Kraków), 4–6 September 1969

The 50th anniversary of the Polish Chemical Society (founded 1919) will be celebrated by the National Congress which will be held in Cracow (Kraków) between 4 and 6 September 1969.—The scope of the Congress will be:

- Chemistry of Solids
- Electrochemistry
- Molecular Spectroscopy
- Chemistry of Complexes
- Analytical Chemistry
- Heteroorganic Chemistry
- Petro- and Carbo-Chemistry
- Macromolecular Chemistry

The Meetings in the Sections will be opened by plenary invited lectures.

The foreign Honorary Members of the Polish Chemical Society will be cordially invited to take part in the Congress.

The Chemical Societies of all countries are cordially invited to send their representatives as the participants to the Congress.

All foreign guests can present communications.

REPORTS ON IUPAC ACTIVITIES

IVTH INTERNATIONAL MATERIALS SYMPOSIUM ON THE STRUCTURE AND CHEMISTRY OF SOLID SURFACES

Berkeley, California, 19-21 June 1968

The IVth International Materials Symposium was held at the Berkeley Campus of the University of California from 19-21 June 1968. The subject of the symposium was "The Structure and Chemistry of Solid Surfaces". The meeting was sponsored jointly by the Inorganic Materials Research Division of the Lawrence Radiation Laboratory and the Department of Chemistry at the University of California at Berkeley. The Co-Chairmen of the conference were Prof. G.A.SOMORJAI, Prof. R.GOMER and Prof. R.F.WALLIS. There were 84 papers presented in two parallel sessions. More than 450 participants from 15 countries attended the lectures.

The main topics of the meeting were reports on the experimental and theoretical studies of the structure of clean surfaces. The experimental techniques included low energy electron diffraction, and field emission microscopy. Reports on gas-surface interactions included studies of molecular beam scattering from surfaces and investigations of surface reactions.

VTH INTERNATIONAL SYMPOSIUM ON THE CHEMISTRY OF NATURAL PRODUCTS

London, 8-13 July 1968

The 10 plenary lectures were given in the lecture theatre of the Royal Garden Hotel. At Imperial College there were seven parallel sessions covering physical methods including X-ray crystallography; naturally occurring compounds containing metals; biosynthesis; proteins and enzyme systems as related to organic chemistry; other macromolecules of biological importance; terpenes and steroids; alkaloids; and other topics in natural product chemistry. Over 300 short papers were delivered, covering the whole range of natural products.

A feature of many of the plenary lectures was the emphasis placed on macromolecules, particularly proteins and nucleic acids; the lectures by E.LEDERER and by Academician M.M.SHEMYAKIN both dealt with the determination of the sequence of amino acids in peptides. The various methods for achieving volatility of the compounds were discussed in detail, as well as the particular problems presented by special amino acids such as arginine and methionine. Applications to the determination of the structure and purity of individual peptides were presented.

Two other plenary lectures dealt with proteins. That given by B.KEIL dealt with the tertiary structure of trypsinogen and chymotrypsinogen and particularly the location of the active and binding sites with respect to the mode of action. The nature of the pancreatic trypsin inhibitor was also discussed to illustrate the nature of enzyme interactions. The lecture by C.B.ANFENSEN discussed staphylococcal nuclease and its possible total synthesis. This enzyme, comprising 149 amino-acid units, has been broken down into fragments, all of which have been synthesized, and the problem of combining these fragments to reconstitute the enzyme is currently being studied.

A stimulating lecture by H.G.KHORANA summarized the outstanding contributions he has made to the synthesis of polynucleotides. Careful choice of protecting groups and conditions for condensations led, for example, to the preparation of all of the 64 triribonucleotides containing the "natural" purine and pyrimidine bases. Larger synthetic polynucleotides have been used in basic studies on the genetic code and the discovery of an enzyme capable of joining polydeoxynucleotide chains offers the possibility of the total synthesis of a gene within another year or so.

D. ARIGONI summarized present knowledge of the biosynthesis of terpenes and described the determination of structure and biogenesis of the mould product pleuromutilin. G.STORK discussed the total synthesis of the alkaloid lycopodine with special reference to the control of the stereochemistry at the various chiral centres. Both of these lectures were characterized by the elegance of the chemical reactions employed and of the underlying logic. T.GOTO, the youngest of the plenary lecturers discussed his recent work on the bioluminescence of the luciferins, a group of substances of differing structures, but all possessing this striking property, which was treated in detail both from chemical and physical standpoints.

H.H.INHOFFEN and R.B.WOODWARD both dealt with macrocyclic tetrapyrrolic compounds. The former described his recent work on the chemistry of porphins and chlorins, especially certain of the oxidation products and the nature of their rearrangement reactions. Prof. WOODWARD, in the concluding plenary lecture, discussed at length (three hours) the present state of his gargantuan total synthesis of vitamin B₁₂ which is being carried out jointly with Prof. A.ESCHENMOSER of Zurich. In the expectation of the happy conclusion of this task, the Conference committee had adopted a simplified version of the B₁₂ structure as its symbol and their optimism was justified in that Prof. WOODWARD was able to announce the closure of the cobalt macrocycle but, alas, through an oxygen bridge rather than through carbon. The conference was officially opened by an introductory address by Lord TODD, and closed after a short speech by Sir EWART JONES.

The ample chemical diet was rendered the more digestible by a variety of social functions including a reception at the Geological Museum, a dinner at the Royal Academy, and other receptions kindly provided by Imperial College, the University of London, ICI, Ciba and Shell. The delegates dispersed at the end of the week with the knowledge that only two years were available to make the discoveries which would justify their visit to the Sixth International Symposium on the Chemistry of Natural Products in Riga in 1970, which will be organized by our Russian colleagues. A.W.JOHNSON

VITH INTERNATIONAL SYMPOSIUM ON THE REACTIVITY OF SOLIDS

Schenectady NY (USA), 25-30 August 1968

The Symposium was attended by about 200 scientists, with some wives attending also. About one-half of these came from countries other than the United States. The meeting was well organized from the standpoints of both the scientific and social programs. Prof. J.W.MITCHELL (University of Virginia) and Drs R.W.ROBERTS and P.CANNON (both General Electric Co.) are to be congratulated on the very evident success achieved in both of these aspects. It was unfortunate that the speakers from Bulgaria, Romania,

Hungary, and the USSR were unable to attend. There is obviously a great amount of scientific interest in reactivity of solids, and this symposium is an excellent medium for catalyzing this interest and acquainting the scientists with each other.

W.S.HORTON, Chief High
Temperature Chemistry Section

IUPAC-SYMPOSIUM ON VALENCE ISOMERIZATION

Karlsruhe (Germany), 9-12 September 1968

The Symposium had been organized by Gesellschaft Deutscher Chemiker and sponsored by IUPAC.

The program included 8 plenary lectures given by: H. SCHMIDT (Switzerland), R. SRINIVASAN (USA), J. F. M. OTH (Belgium), E. VOGEL (Germany), R. B. WOODWARD (USA), F. A. L. ANET (USA), H. M. FREY (Great Britain) and W. VON E. DOERING (USA). These lectures lasted normally 1 to 1½ hours, in an exceptional case 5 hours, however. Besides the plenary lectures 27 short communications have been presented. Each short communication was followed by a 10-minute discussion. In the whole 35 papers have been presented from 12 different countries, under the chairmanships of E. VOGEL (Germany), S. MASAMUNE (Canada), J. A. BERSON (USA), H. SCHMIDT (Switzerland), H. KLOOSTERZIEL (Holland), H. M. FREY (Great Britain) and W. VON E. DOERING (USA).

The Symposium was put into session by Prof. R. CRIEGEE (Karlsruhe), the chairman of the Scientific and Organizing Committee. 250-300 participants took part into a very active and highly interesting scientific program, which did not leave too much time for social events. There was a reception on Tuesday afternoon given by the mayor of the city of Karlsruhe to all the speakers of the Symposium and to invited guests. 100 participants joined a bus tour to a castle in the Black Forest on Wednesday evening.

ANALYTICAL CONFERENCE

Warsaw, 10-14 September 1968

The opening ceremony was held in the morning 10 September, Tuesday, in the Great Hall of the Warsaw Polytechnic. The Chairman of the Organizing Committee, Prof. WIKTOR KEMULA, gave an opening address, followed by the inaugurational address given by Deputy Prime Minister of the People's Republic of Poland, Mr. E. SZYR, under whose patronage the Conference was held. The following welcoming address were given by Prof. J. GROSZKOWSKI, President of the Polish Academy of Sciences, Prof. I. P. ALIMARIN of Moscow University, as the official IUPAC representative, Prof. T. URBAŃSKI, President of the Polish Chemical Society, and Prof. D. SMOLEŃSKI, President of Warsaw Polytechnic.

The program covered all branches of analytical chemistry. The plenary lectures were given during the morning sessions and were dealing with fundamental achievements in analytical chemistry or were presenting the work of some outstanding Polish scientific centers.

These were the following:

- Prof. G. CHARLOT (France): «Le rôle de la chimie analytique dans la recherche pure et appliquée»

- Prof. I. P. ALIMARIN and J. A. ZOLOTOV (USSR): "The use of solvent extraction for concentration of trace elements" (in Russian)
- Prof. D. HUME (USA): "Problems of environmental trace analysis"
- Prof. L. ERDEY (Hungary): "Gravimetry as the basis of chemical analysis"
- Prof. W. KEMULA (Poland): "The application of chromatopolarography to the analysis of the mixtures of organic compounds"
- Dr A. BUDZYŃSKI and J. Z. BEER (Poland): "Determination of biologically important low molecular compounds by radiopaper chromatography"
- Doc. M. WROŃSKI (Poland): "Application of thiomercurimetric titrations to trace analysis"
- Dr R. DYBCZYŃSKI (Poland): "Some factors influencing the quality of separation of chemically similar elements by ion exchange chromatography"

The first five of the above plenary lectures, as well as these of the lectures invited by the Organizing Committee, who could not attend to the Conference, i.e. Prof. R. BELCHER, Dr J. JANAK, and Mr A. JONES will be published in the special issue (Sept.-Oct. 1968) of the Polish journal "Chemia Analityczna" in their original languages.

The 198 discussion papers were grouped in 4 main sections devoted to fundamental problems of analytical chemistry, analysis of inorganic materials, analysis of organic materials and technique of analytical chemistry. For each paper 15 minutes were allotted including time for discussion. These papers were presented in the following languages: Polish 57, English 53, German 51, Russian 29, French 8. The abstracts were prepared as a special issue and were distributed to the participants.

During the Conference the participants had an opportunity to visit the Institute of General Chemistry in Warsaw.

Besides the academic program a party was organized for all participants in the Warsaw Philharmony Building on 10 September, Tuesday. Also the outstanding Polish and foreign scientists were invited for a cocktail party by the Minister of Chemical Industry, on Wednesday, 11 September, and by Deputy Prime Minister on 13 September, Friday. The social program included also sight-seeing tours in Warsaw and vicinity and an excursion to Zelazowa Wola, the birthplace of Chopin, with a piano concert and dinner in the old inn.

The Conference was attended by 602 members including 130 from abroad: Bulgaria, Czechoslovakia, Finland, France, Germany, Hungary, India, Italy, Japan, Rumania, United Kingdom, USSR, Yugoslavia.

V.5. COMMISSION ON ELECTROANALYTICAL CHEMISTRY

Minutes of the Meeting

Date: 30 and 31 August, 1967

Present: Prof. W. KEMULA (Chairman), Dr P. ZUMAN (acting as Secretary), Prof. I. M. KOLTHOFF, Prof. G. CHARLOT, Prof. N. TANAKA, Prof. L. MEITES (Associate Member), Prof. T. FUJINAGA (part time), Prof. E. BISHOP (Observer).

(1) Minutes of Meeting in Paris 1965

The minutes of the meeting in Paris 1965, already approved by circulation, were tabled. In the absence of the Secretary, Prof. R. A. ROBINSON, Dr ZUMAN accepted the invitation to be acting Secretary. Profs G. CHARLOT, N. TANAKA and Dr R. G. BATES remained liaison officers with Commission I.3 (Commission on Electrochemistry of the Division of Physical Chemistry).

(2) *Publication Activities*

(i) *Dissociation Constants of Inorganic Acids and Bases in Aqueous Solutions.*—Dr D. D. PERRIN submitted a manuscript on Dissociation Constants of Inorganic Acids and Bases in Aqueous Solutions, which was approved by Prof. I. M. KOLTHOFF, Prof. R. A. ROBINSON and Dr R. G. BATES. The Commission recommended the report for publication and the manuscript was handed over to the Division Secretary for publication in *Pure and Applied Chemistry* and/or as a monograph.

(ii) The report by P. DELAHAY, G. CHARLOT and H. A. LAITINEN published in the Information Bulletin was recommended for publication in *Pure and Applied Chemistry* without change.—The report by R. G. BATES on “A Proposal for the Practical Measurement of pH in Amphiprotic and Mixed Solvents” published in the Information Bulletin was also recommended for publication in *Pure and Applied Chemistry*.

Two motions were recommended to the Division Committee: (1) We suggest that the Chairman and/or Secretary of a Commission submitting a report be informed by the Publication Committee when it has been accepted for publication. (2) We suggest the opportunity be given to an author to bring his report up to date if it is being published more than one year after it had been submitted. No report should be published without the author's approval of the proofs.

(3) *Tables of Oxidation-Reduction Potentials*

The Commission agreed that the Tables of Oxidation-Reduction Potentials by G. CHARLOT prepared in 1955 are out of date and that a new set of tables be prepared and published. Prof. G. CHARLOT agreed to prepare the tables together with his co-workers.

(4) *Purification of Solvents*

The Subcommission on Purification of Solvents headed by Prof. G. CHARLOT received and approved the reports by L. A. KNECHT on “Purification of N-Methylacetamide and Test of Purity” and by L. MUKHERJEE and S. BRUCKENSTEIN on “Purification of Ethylenediamine”. These reports are being recommended for publication. Reports by G. KORTUM on “Purification of Hydrocyanic Acid”, by T. B. REDDY on “Purification of Dimethylsulfoxide for Electrochemical Experimentation” and by Mme BADOZ-LAMBLING on “Purification of Tetrahydrofuran” are being re-edited. The project of purification of formamide and its derivatives is dealt with in cooperation with M. SPIRO. Prof. G. CHARLOT will prepare a list of solvents important in analytical chemistry and will suggest authors who could prepare a report on their purification. The list will be sent to all members of Commission V.5 for suggestion on solvents and authors. The publication of all reports in one volume was discussed. The report by L. A. KNECHT was selected as model sample and other reports should be organized similarly.

(5) *Electrochemistry in Non-Aqueous Media*

The Sub-Commission on Electrochemistry in Non-Aqueous Media headed by I. M. KOLTHOFF received a preliminary report by J. F. COETZEE and C. E. WILSON on “Standard and Formal Potentials in Acetonitrile”. A report by L. MUKHERJEE and S. BRUCKENSTEIN on “Standard and Formal Potentials in Ethylenediamine” is in preparation. The work on ion mobilities, standard and reference electrode potentials, equilibrium constants and mean activity coefficients in non-aqueous systems is continued. Prof. I. M. KOLTHOFF will prepare a list of values of dissociation constants of uncharged and monovalent cation acids in acetonitrile.

(6) *Polarographic Data*

The Sub-Commission on Polarograph Data headed by P. ZUMAN reported on the progress of work on the collection of half-wave potentials of inorganic systems (Dr A. A. VLČEK). Prof. L. MEITES indicated the possibility of financial support in the US for the collection of polarographic data. It was suggested that the Division Committee ask the Bureau of the IUPAC whether there is any cooperation between the IUPAC on the one hand and the Reference Data System (Washington, DC, USA) or/and the equivalent Russian system on the other hand regarding the compilation and further handling of critically selected data. The exchange of information between existing organizations publishing polarographic bibliographies will be encouraged. Prof. L. MEITES will contact the Sargent Company to find out whether they plan to prepare a new edition of their bibliography. The KWIC indexing will be investigated at a later stage. Prof. T. FUJINAGA reported on the progress of Polarographic Data Cards. Help was promised when requested. The Secretary will inform the Polarographic Societies of Britain and Japan on the organization of a polarographic congress in 1969 in Italy. Prof. MEITES suggested the possibility of critical evaluation of selected polarographic procedures. He will report at a later date.

(7) *Purification and Purity of Reagents Used in Electroanalytical Chemistry*

The Sub-Commission on Purification and Purity of Reagents Used in Electroanalytical Chemistry headed by W. KEMULA will follow the work by Z. GALUS on "Purification and Purity of Supporting Electrolyte Solutions". L. MEITES will report on possible methods of purification of mercury for electroanalytical purposes.

(8) *Solid Electrodes*

A Sub-Commission on Limitations and Applications of Solid Electrodes in Electroanalytical Chemistry was created (Prof. N. TANAKA and E. BISHOP). It will deal with recommendations for pre-treatment of platinum electrodes for various purposes and with compilations on chronovoltammetric E_p and $E_{P/2}$ data.

(9) *Nomenclature*

At the suggestion of Prof. G. CHARLOT it was recommended that the Commission pay more attention to problems of nomenclature, terminology and standardization.

A summarising list of activities of all Commissions of Division V should be published by the Division Committee in analytical journals.

In order not to interrupt the meetings of Commissions, the Division Committee should meet on the day before and on the day after the meetings of the Commissions.

(10) *Symposium*

A motion was submitted and passed that a Symposium on "Non-Aqueous Electrochemistry" be sponsored jointly by our Commission and Commission I.3.

Submitted to the Secretary of Division V on November 14 1967.

I. M. KOLTHOFF
Chairman, Commission V.5

IUPAC COMMITTEE ON THE TEACHING OF CHEMISTRY

Workshop on Evaluation of Chemistry Courses at School Level

Peradeniya University (Ceylon), 13-18 August 1968

The Workshop was organized by the IUPAC Committee on the Teaching of Chemistry and sponsored by the Ministry of Education, Ceylon, and UNESCO.

There were 10 participants from countries outside Ceylon and a further 10 from the University, Teachers' College and the Ministry of Education Science Project in Ceylon.

The aim of the Workshop was to follow up the IUPAC Report on "The Effect of Examinations in Determining Chemistry Curricula" and to consider particularly how the administration and construction of chemistry examinations could be designed to produce a desired effect on the teaching of chemistry within an educational system. Special thought was given to the problems of introducing new curricula in chemistry in developing countries.

The Workshop was held in Ceylon in order to utilize the experience of the team in the Ministry of Education in that country, who have been working on new chemistry examinations for some years. The examples chosen for study were based on those questions and test items produced at a Teacher Educators' Seminar held in Ceylon just before the International Workshop.

The Workshop was under the Chairmanship of Prof. H. F. HALLIWELL (UK); Mr J. C. MATTHEWS, the author of the original IUPAC Report, was among the participants, and Mr D. G. CHISMAN, Secretary, IUPAC Committee on the Teaching of Chemistry, acted as Secretary to the Conference. Financial assistance for visiting participants was made available by various national authorities and by UNESCO.

A report of the Workshop with supporting papers is being prepared and will be published, probably by UNESCO, in 1969.

17 October 1968

D. G. CHISMAN

TENTATIVE

IUPAC/IUB 1967 REVISED RULES FOR NOMENCLATURE OF STEROIDS*[†]

Rule	Contents	Page
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2S-1	General	25
2S-2	Fundamental carbocycles	30
2S-3	Penta- and sexi-cyclic modifications	35
2S-4	Derivatives	44
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Introduction

The rules of steroid nomenclature originate from a discussion held at the Ciba Foundation in London, England, in 1950 between the representatives of many schools. These were published in *Chemistry and Industry*, 1951, 23 Jan., pp.SN 1-11, and also in French and German. They were subsequently taken over by the International Union of Pure and Applied Chemistry and published in an official form in the *Comptes rendus* of the Zurich meeting in 1952 (also IUPAC Nomenclature of Organic Chemistry, Sections A and B, 1957, 1st edn 1958; 2nd edn 1966, pp.71-82, Butterworths, London; and numerous reprints and translations).

In 1960 a group of specialists under the chairmanship of Prof. T. REICHSTEIN, including representatives of the IUPAC Commissions of the Nomenclature of Organic Chemistry and of Biochemical Nomenclature, met in Basle, Switzerland, for discussions of amendments and additions to the Rules. Agreement was not reached on all the points discussed, and the results of this meeting were therefore published in discussion form in the *IUPAC Information Bulletin*, No.11. They have generally been referred to as the "Basle Proposals".

* These Rules shall be known as the IUPAC/IUB 1967 Revised Tentative Rules for Steroid Nomenclature.

[†] These Rules are issued by the IUPAC Commission on the Nomenclature of Organic Chemistry [P. E. VERKADE (Chairman), L. C. CROSS, G. M. DYSON, G. KERSAINT, K. L. LOENING, N. LOZACH, H. S. NUTTING, S. VEIBEL; Associate members, R. S. CAHN, J. RIGAUDY; Observers, K. A. JENSEN, W. KLYNE], and by the IUPAC/IUB Commission of Biochemical Nomenclature [O. HOFFMANN-OSTENHOF (Chairman), A. E. BRAUNSTEIN, W. E. COHN, J. S. FRUTON, B. KEIL, W. KLYNE, C. LIEBECQ, M. G. MALMSTRÖM, R. SCHWYZER, E. C. SLATER; Corresponding member, N. TAMIYA; Observer, S. VEIBEL].

Since then, many points in the Basle proposals have become almost universally accepted in the literature. In 1965 the two International Commissions concerned, namely, the IUPAC Commission of the Nomenclature of Organic Chemistry and the Commission on Biochemical Nomenclature (now jointly responsible to IUPAC and IUB), decided that the time had come for as many as possible of the Basle Proposals to be formulated as rules.

The present Rules include: all the original Rules, mostly renumbered (with additions and amendments arising from the Basle Proposals or from current practice in the literature); and most of the Basle Proposals, namely, those which have been generally accepted. Further, adoption of the sequence-rule procedure* for general stereochemical descriptions in much of the chemical literature has permitted its introduction now also for some sections of steroid nomenclature that were previously in dispute or intractable. Decisions on a few of the Basle Proposals have, however, been postponed; it is hoped that further experience will indicate the most appropriate ways of dealing with them.

General Application

Although these Rules are called "Rules for Nomenclature of Steroids", many of the principles therein have become almost universally accepted also in diterpene and triterpene chemistry; also to some extent for sesquiterpenes and for several groups of alkaloids. It is suggested that the same principles may be applied to a number of other specialized groups of natural products, perhaps without the need for further official rules, so long as the basic ideas are followed. These principles include: (i) clear definition of stem names and the stereo-chemistry implied in them; (ii) systematic application of the rules of general organic chemical nomenclature, with modifications where special considerations make this necessary; (iii) application of the methods of skeletal modification given in these Rules, viz., the use of homo and nor for, respectively, stepwise expansion and contraction of ring systems; the use of *seco* for reductive fission of ring systems; and the use of *abeo* for formal bond migrations (this flexible concept was first proposed by Prof. D.H.R. BARTON at an informal meeting of terpene chemists convened by the Chemical Society in London, England).

Comments

Comments on these Tentative Rules should be sent to:

Prof. P. E. VERKADE
Ary Schefferstraat, 217, 's-Gravenhage
(Netherlands)

or Prof. O. HOFFMANN-OSTENHOF
Biochemische Abteilung
Lehrstuhl für Biochemie der Universität Wien
Währinger Strasse 68, 1090 Vienna
(Austria)

or to any member of the Commissions named in the footnote on page 23.

* R.S. CAHN, (Sir) CHRISTOPHER INGOLD, and V. PRELOG, *Angew. Chem.*, internat.edn, 5, 385 (1966) (in English); *Angew. Chem.*, 78, 413 (1966) (in German). For a partial simplified account see R.S. CAHN, *J. Chem. Educ.*, 41, 116 (1964).

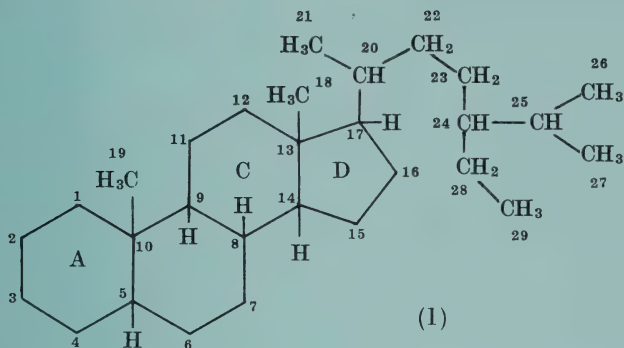
RULES

Rules are numbered 2S-1, 2S-2, 2S-3, etc., the first "2" denoting that this is the second or revised set of rules. The numbers of the corresponding previous rules, where they exist, are included for comparisons.

General

Rule 2S-1 (Expanded from Rules S-1 and S-2)

1.1 Steroids are numbered and rings are lettered as in formula (1). If one of the two methyl groups attached to C-25 is substituted it is assigned the lower number (26); if both are substituted, that carrying the substituent

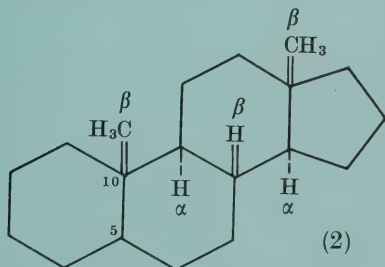


cited first in the alphabetical order or order of complexity is assigned the lower number (cf. IUPAC 1965 Rule* C-15.11 (e)). For trimethyl steroids see Rule 2S-2.3, Note 2.

1.2 If one or more of the carbon atoms shown in (1) is not present and a steroid name is used, the numbering of the remainder is undisturbed.

1.3 For a steroid the name, including stereochemical affixes, and its structural formula (see Rule 2S-1.4), denote the absolute configuration at each asymmetric centre (see also Rule 2S-1.5). When the configuration at one or more centres is not known, this is indicated by Greek letter(s) ξ (xi) prefixed by the appropriate numeral(s).

1.4 When the rings of a steroid are denoted as projections on to the plane of the paper, the formula is normally to be orientated as in (2). An atom or group attached to a ring depicted as in the orientation (2) is termed α (alpha)

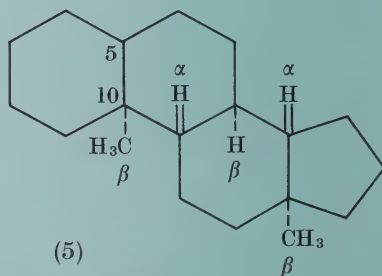
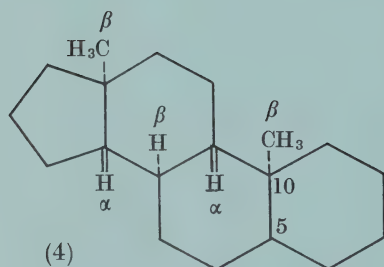
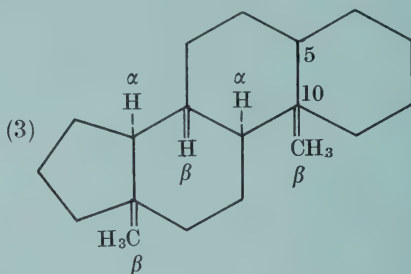


* IUPAC Nomenclature of Organic Chemistry, Section C, 1965, Butterworths, London.

if it lies below the plane of the paper or β (beta) if it lies above the plane of the paper. In formulae, bonds to atoms or groups lying below the plane of the paper are shown as broken (---) lines, and bonds to atoms or groups lying above the plane of the paper are shown as solid lines (preferably thickened **▬**). Bonds to atoms or groups whose configuration is not known or is unspecified are denoted by wavy lines (~).

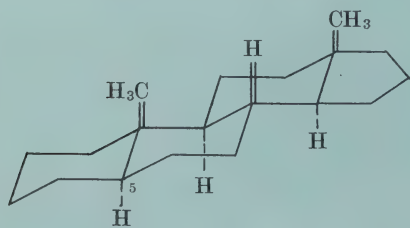
Notes

- (1) Projections of steroid formulae should not be orientated as in formula (3), (4), or (5) unless circumstances make it obligatory.

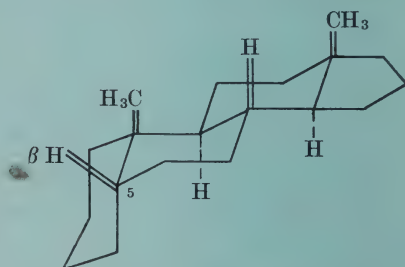


- (2) With the preferred orientation (2), and with (3), α -bonds appear as broken lines and β -bonds as solid (thickened) lines. The reverse is true for (4) and (5). Wavy lines denote ξ -bonds for all orientations of the formula.

- (3) A perspective representation of the stereochemistry of formula (2) as in (2a) or (2b) may also be used.



(2a) A 5α -steroid



(2b) A 5β -steroid

(For the significance of the prefixes 5α - and 5β - see Rule 2S-1.5.)

When steroid formulae are drawn in this way, bonds pointing upwards are, by convention, drawn bold and bonds pointing downwards are drawn broken; these representations correspond to the β - and α -bonds of projection formulae such as (2) and do not conform to the general practice that bold and broken lines denote bonds projecting respectively above and below the plane of the paper. Note, however, that the general practice is followed with chair and boat forms of spirostans (see Rule 2S-3.3).

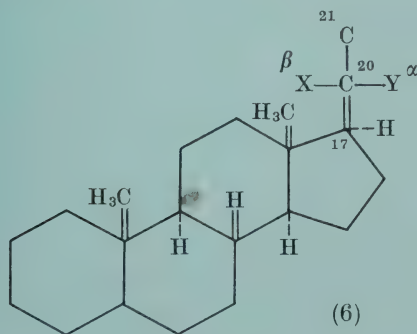
(4) All hydrogen atoms and methyl groups attached at ring junction positions must always be inserted as H and CH₃, respectively (Me may be used in place of CH₃ if editorial conventions require it). The practice, sometimes followed, of denoting methyl groups by bonds without lettering is liable to cause confusion and should be abandoned. This is essential in view of customs in other fields and applies also to other groups of compound such as cyclic terpenes and alkaloids for which steroid conventions are commonly used.

1.5 Unless implied or stated to the contrary (see Rules 2S-3, 2S-4.4, 2S-5, and 2S-11), use of a steroid name implies that atoms or groups attached at the ring-junction positions 8, 9, 10, 13, and 14 are orientated as shown in formula (2) (*i.e.*, 8 β , 9 α , 10 β , 13 β , 14 α), and a carbon chain attached at position 17 is assumed to be β -oriented (see Notes below). The configuration of hydrogen (or a substituent) at the ring-junction position 5 is always to be designated by adding α , β , or ξ after the numeral 5, this numeral and letter being placed immediately before the stem name. The configuration of substituents attached at other centres of asymmetry in the tetracyclic system A-D is stated by adding α , β , or ξ after the respective numerals denoting their position.

Notes

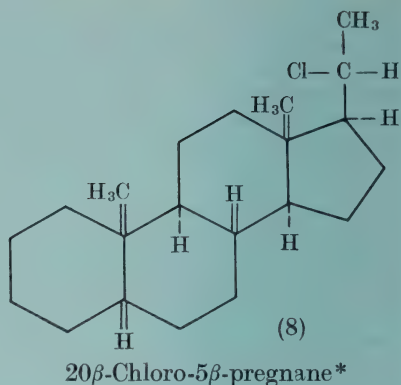
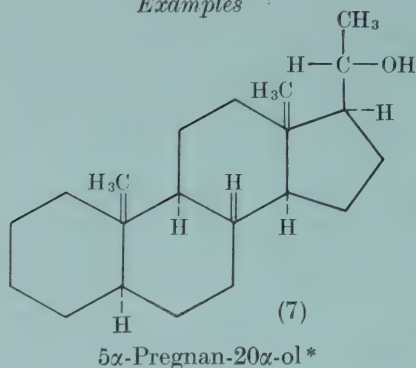
For the purpose of this Rule a carboxyl group at position 17 is not considered to constitute a carbon "chain" (for the nomenclature used see Rule 2S-4.3). For penta- and sexi-cyclic derivatives see Rule 2S-3, and for stereochemical modifications see Rule 2S-5.

1.6 When the configuration at position 20 in the side chain of a pregnane derivative* is as depicted in the projection formula (6) (*i.e.*, a Fischer projection but with the highest number at the top), substituents shown to the right of C-20 are termed α and those to the left are termed β .



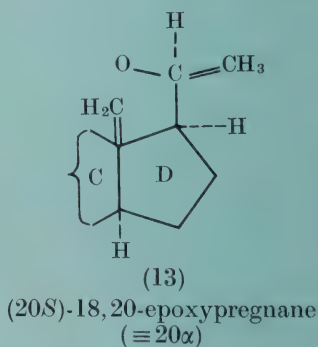
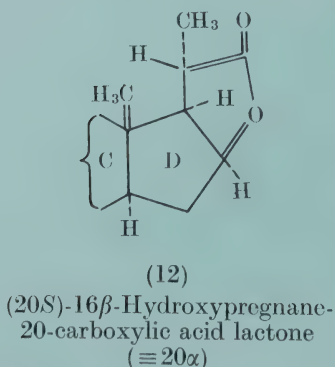
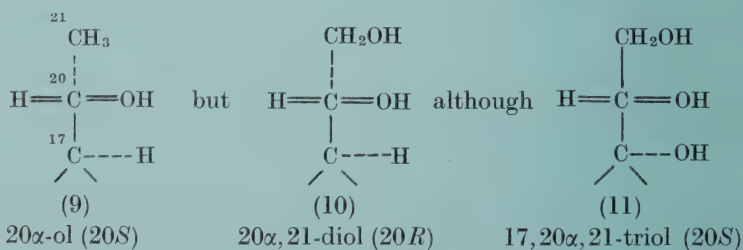
* For the name "pregnane" see Rule 2S-2.3.

Examples :



Notes

(1) The 20 α /20 β -nomenclature is continued because of long tradition. When a longer side chain is present at C-17 the sequence-rule procedure (see ref. 1) is more generally convenient (see Rule 2S-1.7) and it may also be used to designate stereochemistry at C-20 in pregnanes, being particularly useful for 20-substituents that may cyclize with a substituent at another position [*e.g.*, carboxylic acids as in example (12)]. For 20-hydroxy-, 20-alkoxy-, 20-acyloxy-, 20-amino-, and 20-halogeno-derivatives of pregnane without a substituent on C-17 or C-21, 20 α - is equivalent to (20*S*)-, and 20 β - to (20*R*)-; however, these equivalences are sometimes reversed when additional substituents are present, *e.g.*, on C-17 or C-21, and in such cases reference 1 should be consulted.

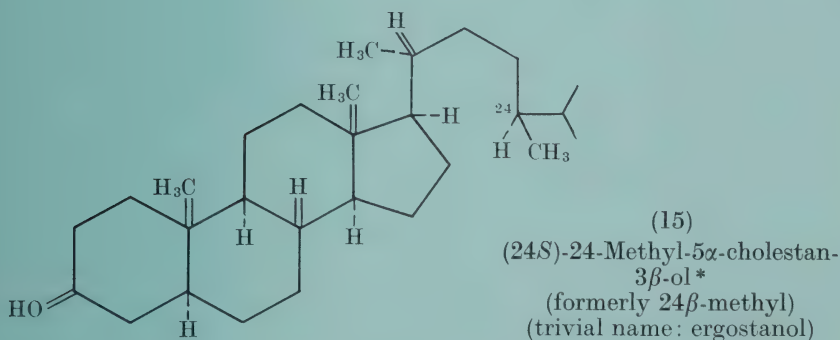
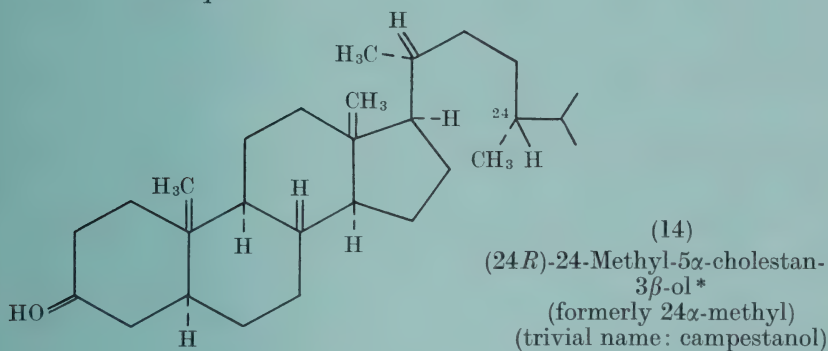


* For the name "pregnane" see Rule 2S-2.3.

(2) When stereochemistry at C-20 is denoted by a Fischer-type projection, as in (6)–(11) or for cardenolides as (37) or bufanolides as (43), the 17,20-bond is preferably denoted by an ordinary line: the stereochemistry at C-17 is then adequately denoted by a thick or a broken bond to the H or to the other substituent (*e.g.*, OH) at position 17. In such formulae, representing the 17,20-bond by a thick or a broken line cannot be correct for both C-17 and C-20; this has, however, frequently been done, then involving the additional convention that the way in which this bond is written is neglected when considering the stereochemistry at C-20.

1.7 The stereochemistry at C-20 and other positions in steroid side chains longer than ethyl is described by the sequence-rule procedure (ref. 1).

Examples



Notes

(1) The sequence-rule procedure is also used when the side chain is cyclized (see Rules 2S-3.3 and 2S-3.4).

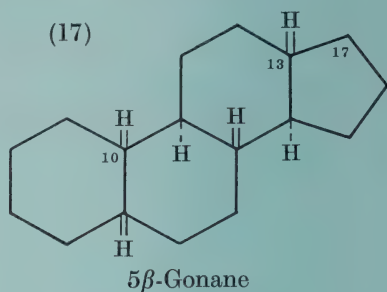
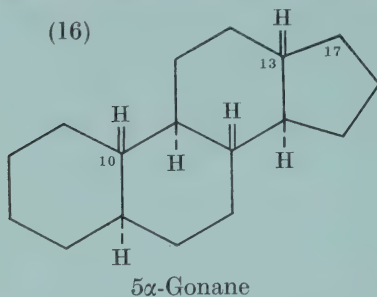
(2) The backbone of a 17-side chain is best denoted as in the plane of the paper (lines of ordinary thickness), the 17,20-bond being similarly denoted. Except for pregnane derivatives, stereochemistry due to substituents on the chain is then indicated by the customary thick or broken lines denoting bonds that project, respectively, above and below the plane of the paper.

* For the name "cholestane" see Rule 2S-2.3. These systematic names are preferred to the trivial names given below them.

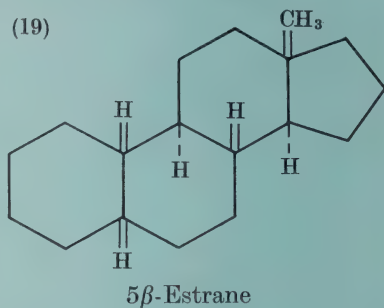
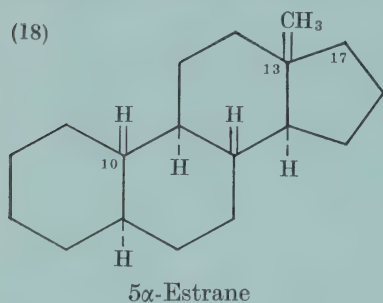
Fundamental carbocycles

Rule 2S-2 (Expanded from Rules S-3.1 to S-3.5)

2.1 The parent tetracyclic hydrocarbon without methyl groups at C-10 and C-13 and without a side chain at C-17 is named "gonane".



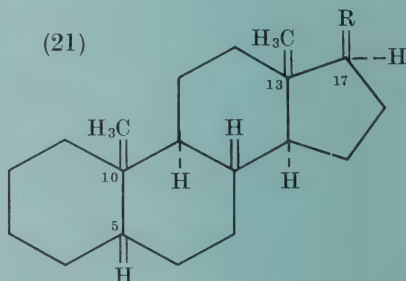
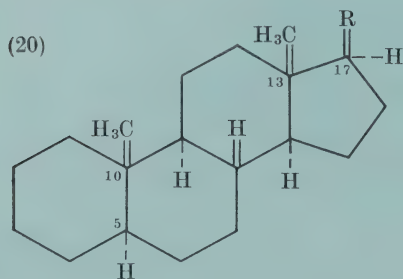
2.2 The hydrocarbon with a methyl group at C-13 but without a methyl group at C-10 and without a side chain at C-17 is named "estrane".



Note

Names of compounds having a methyl group attached to C-10 and a hydrogen atom attached to C-13 are to be based on 18-norandrostane (see Rules 2S-2.3 and 2S-7.1) and not on 10-methylgonane.

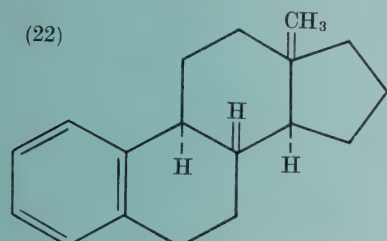
2.3 The following names are used for the hydrocarbons (20) and (21) with methyl groups at both C-10 and C-13.



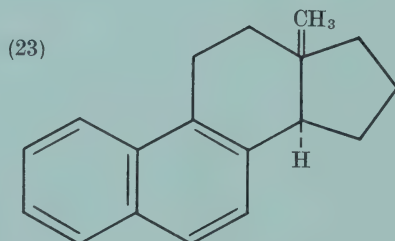
R	(20) 5 α -Series	(21) 5 β -Series
H	5 α -Androstane	{ 5 β -Androstane (not Testane)
C ₂ H ₅	{ 5 α -Pregnane (not Allopregnane)	5 β -Pregnane
*CH(CH ₃)CH ₂ CH ₂ CH ₃	{ 5 α -Cholane (not Allocholane)	5 β -Cholane
*CH(CH ₃)CH ₂ CH ₂ CH ₂ CH(CH ₃) ₂	5 α -Cholestane	{ 5 β -Cholestane (not Coprostate)
^{24Δ} *CH(CH ₃)CH ₂ CH ₂ CH(CH ₃)CH(CH ₃) ₂	5 α -Ergostane	5 β -Ergostane
^{24$\Delta\Delta$} *CH(CH ₃)CH ₂ CH ₂ CH(C ₂ H ₅)CH(CH ₃) ₂	5 α -Stigmastane	5 β -Stigmastane

Notes

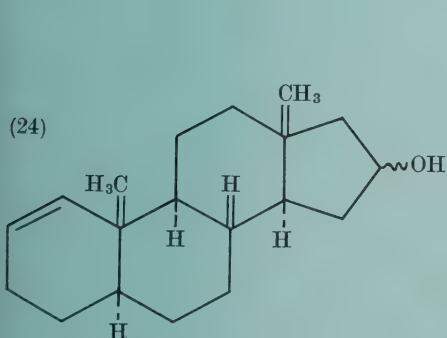
(1) Unsaturation and substituents are denoted in the names of steroids by the usual methods of organic chemistry (cf. Rule 2S-4). Examples (22)–(25) illustrate some simple cases.



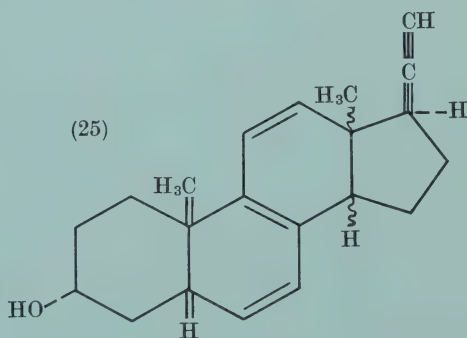
1,3,5(10)-Estratriene



1,3,5(10),6,8-Estrapentaene



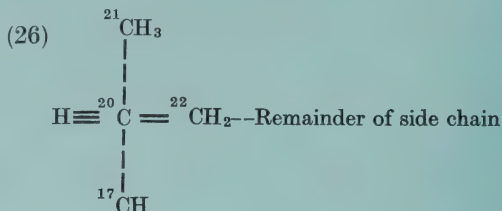
5 α -Androst-1-en-16 ξ -ol



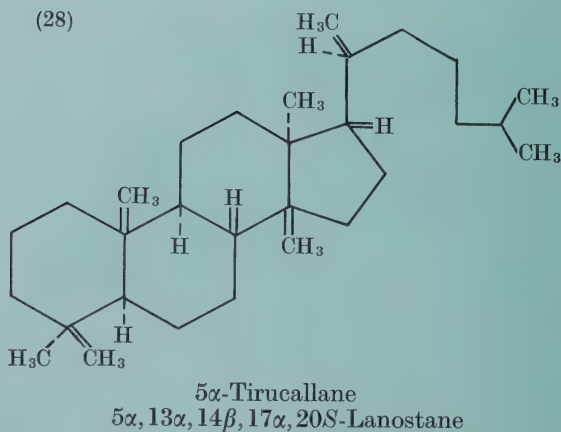
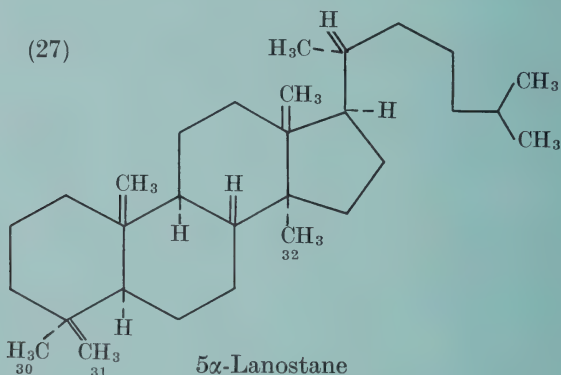
5 β ,13 ξ ,14 ξ -Pregna-6,8,11-trien-20-yn-3 α -ol

* 20*R*-Configuration ◊ 24*S*-Configuration ◊◊ 24*R*-Configuration

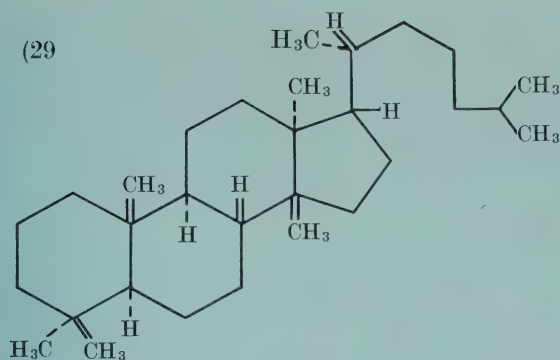
(2) The names "cholane", "cholestane", "ergostane", and "stigmastane" imply the configuration at C-20 shown in partial formula (26); this is (20*R*) except for some derivatives containing additional substituents (cf. Note to Rule 2S-1.6).



(3) Tetracyclic triterpenoids may be regarded as trimethyl steroids, the three additional methyl groups being numbered 30 (attached to C-4 with α -configuration), 31 (attached to C-4 with β -configuration), and 32 (attached to C-14); for example, 5 α -lanostane (27) is 4,4,14 α -trimethyl-5 α -cholestane, the former name implying 14 α ,20*R*-configuration. Trivial names are common in this series of compounds, and some are illustrated in examples (27)–(31).

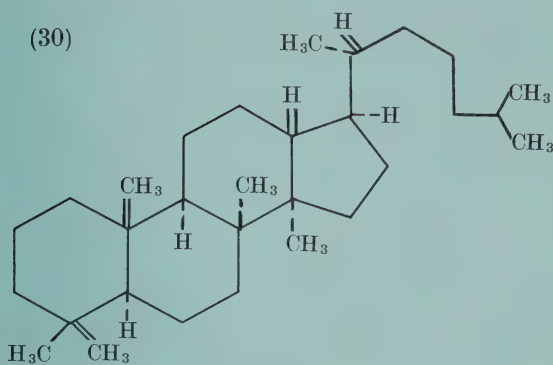


(29)



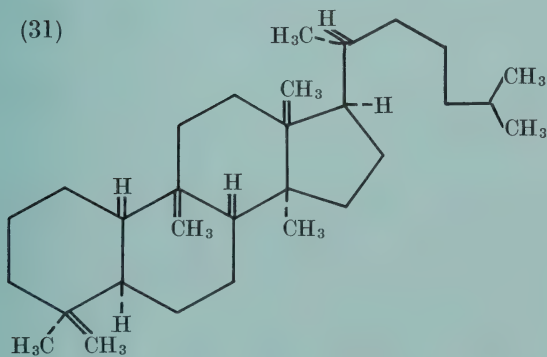
5 α -Euphane
5 α , 13 α , 14 β , 17 α -Lanostane
(20*R* implied in the name)

(30)



5 α -Dammarane
8-Methyl-18-nor-5 α -lanostane
(All configurations except
5 α are implied in the name)

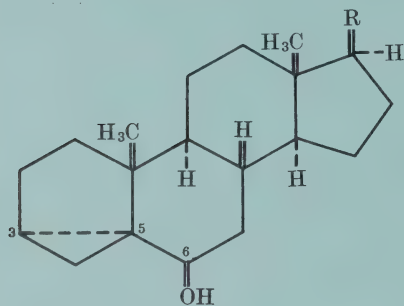
(31)



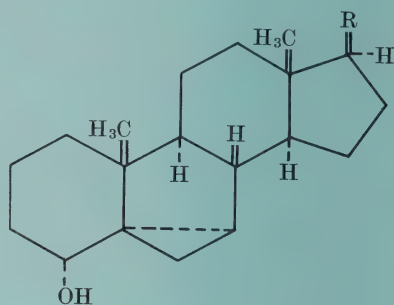
5 α -Cucurbitane
19(10 \rightarrow 9 β)-abeo-5 α -Lanostane
(for the *abeo* nomenclature
see Rule 2S-9)

2.4 When an additional ring is formed by means of a direct link between any two carbon atoms of the steroid ring system or the attached side chain, the name of the steroid is prefixed by "cyclo"; this prefix is preceded by the numbers of the positions joined by the new bond and the Greek letter (α , β , or ξ) denoting the configuration of the new bond, unless that designation is already implicit in the name.

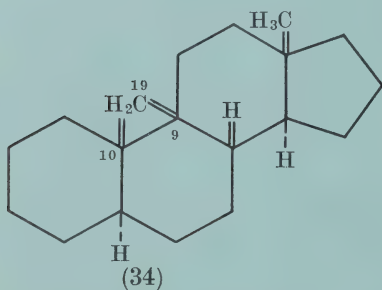
Examples



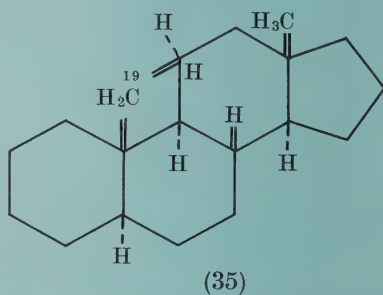
3 α ,5-Cyclo-5 α -cholestan-6 β -ol



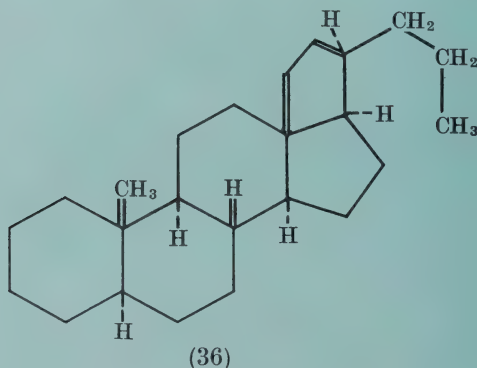
5,7 α -Cyclo-5 α -cholestan-4 α -ol



9,19-Cyclo-5 α ,9 β -androstane



11 β ,19-Cyclo-5 α -androstane



(20*S*)-18,21-Cyclo-5 α -cholane

Penta- and sexi-cyclic modifications

Rule 2S-3 (Amended versions of Rules S-3.6 to S-3.9)

3.1 (a) The name "cardanolide" is used for the fully saturated system (37) of digitaloid lactones whose configuration is as illustrated (the configuration at position 20 is shown as a Fischer-type projection* and is the same as that in cholesterol, *i.e.*, 20*R*). Notwithstanding Rule 2S-1.5, the configuration at position 14 must always be stated as an affix to the names of these compounds.

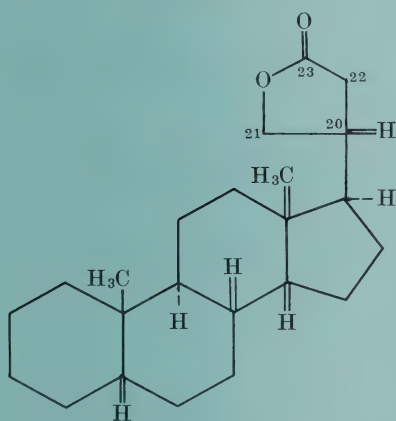
(b) Names such as "20(22)-cardenolide" are used for the naturally occurring unsaturated lactones of this type.

(c) The names "14,21-" and "16,21-epoxycardenolide" are used for the compounds containing a 14,21- or a 16,21-oxygen bridge, respectively.

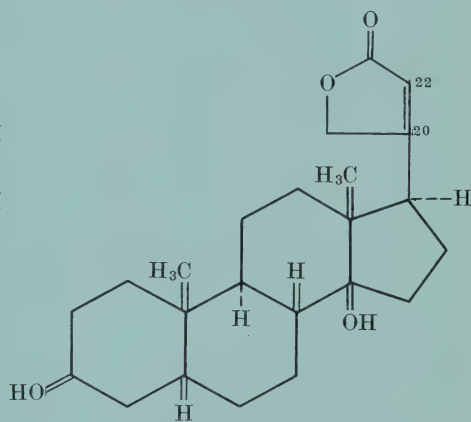
Note

Statement of the configuration at C-14 for all cardanolides is a change from the earlier steroid Rules and is in line with current practice.

Examples



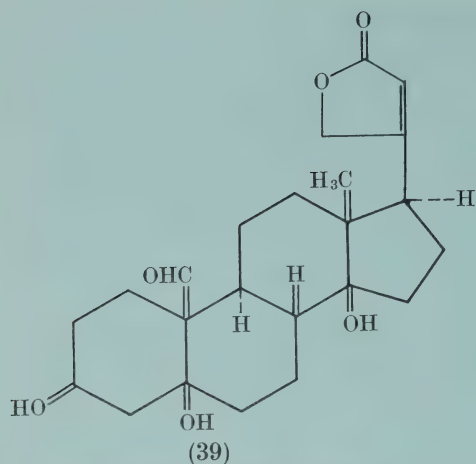
(37)
5β,14β-Cardanolide



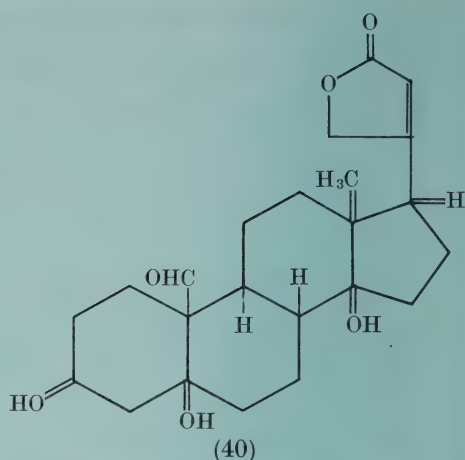
(38)
3β,14-Dihydroxy-5β,14β-card-
20(22)-enolide
(= Digitoxigenin[◊])

* This method of drawing is customary for the steroids. Since the highest-numbered atom is at the top, the usual Fischer projection has been rotated in the plane of the paper through 180°.

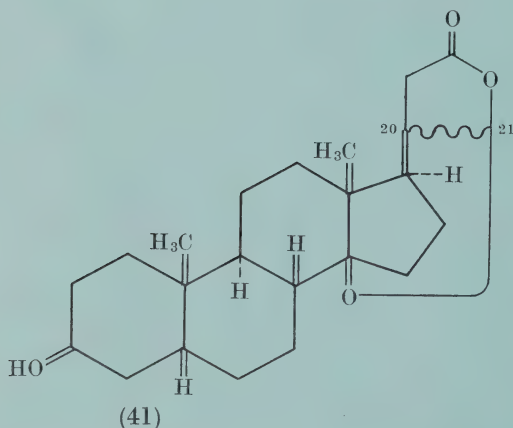
◊ Denotes a trivial name; the systematic name is preferred.



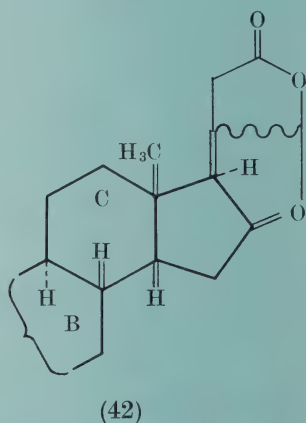
3 β ,5,14-Trihydroxy-19-oxo-5 β ,
14 β -card-20(22)-enolide
(= Strophanthidin*)



3 β ,5,14-Trihydroxy-19-oxo-5 β ,
14 β ,17 α -card-20(22)-enolide
(= 17 α -Strophanthidin*)
(also, allostrophanthidin \diamond)



3 β -Hydroxy-14,21 ξ -epoxy-
5 β ,14 β ,20 ξ -cardanolide
(= Isodigitoxigenin \diamond)



A 16 β ,21 ξ -epoxy-14 β ,20 ξ -
cardanolide

3.2 The name "bufanolide" is used for the fully saturated system (43) of the squill-toad poison group of lactones, with the configuration at position 20 shown (this configuration is drawn as a Fischer-type projection (see Note to Rule 2S-3.1(a)) and is the same as in cholesterol, *i.e.*, 20*R*). Notwithstanding Rule 2S-1.5, the configuration at position 14 must always be stated as an affix to the names of these compounds. Unsaturated derivatives are named by replacing the suffix -anolide by -enolide, -adienolide, etc.; thus, the name "20,22-bufadienolide" is used for the naturally occurring doubly unsaturated lactones.

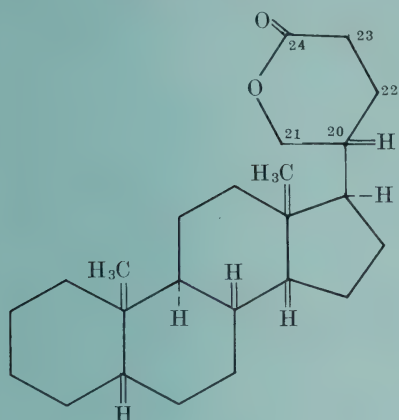
* Denotes a trivial name; the systematic name is preferred.

\diamond Denotes a previous trivial name now considered unacceptable.

Note

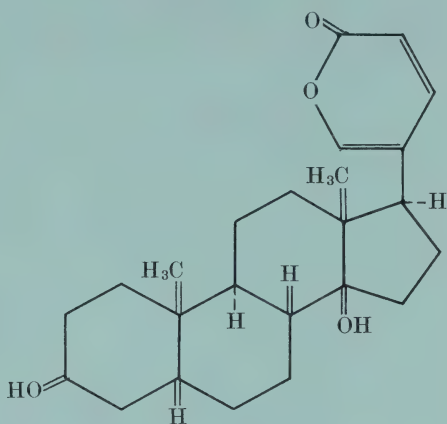
Statement of the configuration at C-14 for all bufanolides is a change from the earlier steroid Rules and is in line with current practice.

Examples



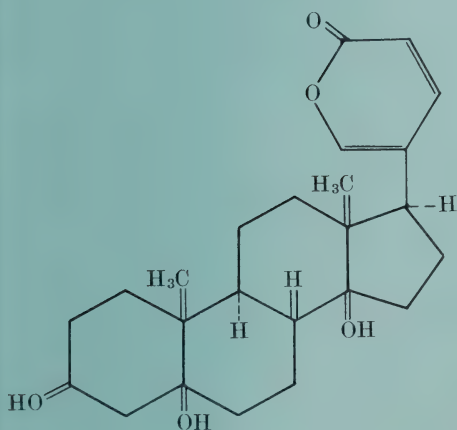
(43)

5β,14β-Bufanolide



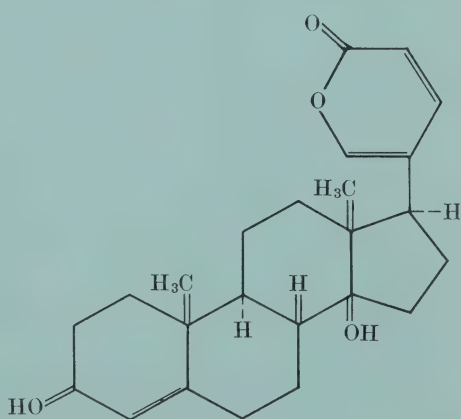
(44)

3β,14-Dihydroxy-5β,14β-bufa-
20,22-dienolide
(= Bufalin*)



(45)

3β,5,14-Trihydroxy-5β,14β-bufa-
20,22-dienolide
(= Telecinobufagin*)



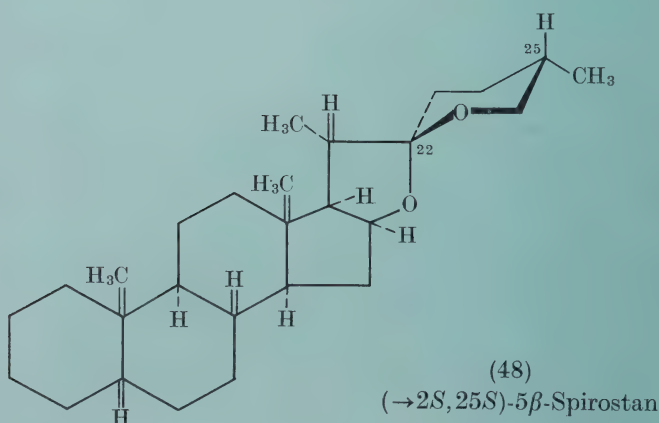
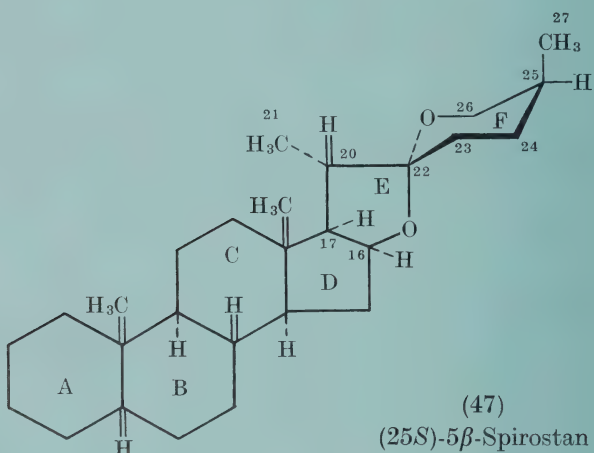
(46)

3β,14-Dihydroxy-14β-bufa-
4,20,22-trienolide
(= Scillarenin*)

* Denotes a trivial name; the systematic name is preferred.

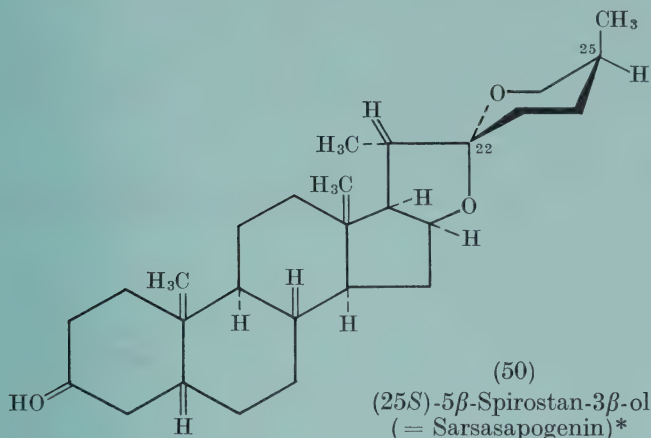
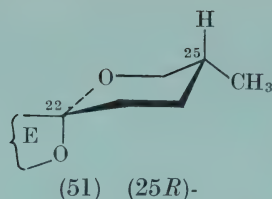
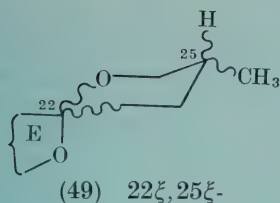
3.3 The name "spirostan" is used for the compound of structure (47)*; this name specifies the configurations shown for all the asymmetric centres except positions 5 and 25. A prefix 5 α - or 5 β - is added in the usual way (see Rule 2S-1.5). Configurations at C-16 and C-17, if different from those shown in formula (47), are designated as 16 β (H) and 17 β (H). Configurations at C-20 and C-22, if different from those shown in formula (47), are designated by the sequence-rule procedure \diamond or, if unknown, by ξ . Steric relations of substituents at C-23, C-24, C-25, or C-26 are in all cases designated by the sequence-rule procedure \diamond or, if unknown, by ξ .

Examples



*This is a 16,22:22,26-diepoxycholestane.

\diamond See ref. 1.



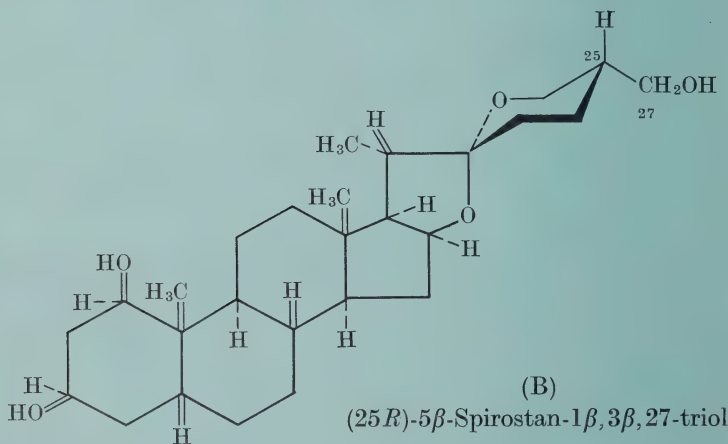
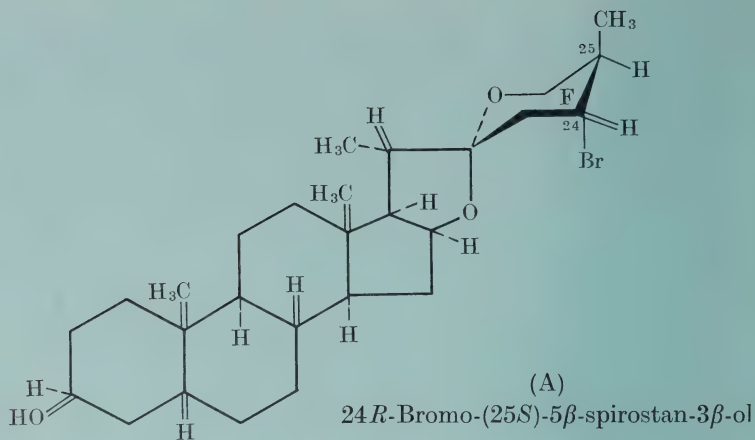
Notes

Several other methods have been used in the past for designating stereochemistry at C-22 and C-25 in the spirostans and related series; all involve serious difficulties (cf. the Basle Proposals, IUPAC *Information Bulletin*, No. 11; also L. F. FIESER and M. FIESER: "The Steroids", Reinhold, New York, 1959, Chapter 21). The sequence-rule procedure is adopted in these Rules because it gives an unequivocal symbolism.

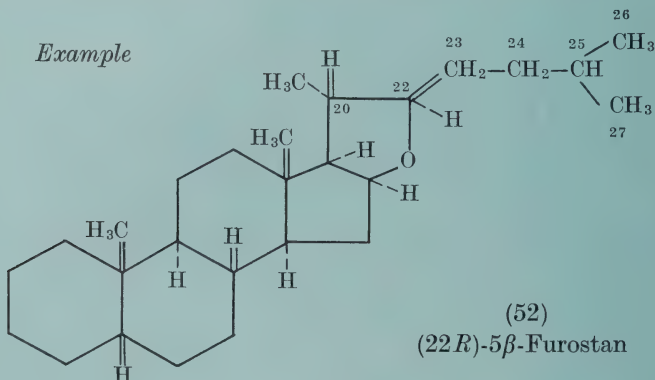
It is to be noted that, although ring E, like rings A, B, C, and D, can conveniently be shown by projection on to the plane of the paper, yet ring F cannot be adequately represented in this way since the oxygen atom, C-26, C-24, and C-23 lie in one plane that is perpendicular to the plane of the paper. Ring F is conveniently drawn as in formulae (47)–(51); in formula (47), for instance, the broken line from C-22 to oxygen denotes that the oxygen atom and C-26 of ring F lie behind the plane of the paper and that consequently C-23 and C-24 lie in front of the plane of the paper (configuration *R* at C-22). In partial formula (48) the configuration at C-22 is reversed and must be stated in the name (*S*). It is conventional to draw ring F as a chair, but this conformation is not implied in the name "spirostan"; whatever the conformation of ring F, C-27 and the 25-hydrogen atom both lie in the plane of the paper and so cannot be denoted by broken or thickened lines or designated α or β . In (47) the methyl group is axial (above the general plane of ring F), and in (48) it is equatorial (in the general plane of ring F); in both these cases the configuration at C-25 is *S*, but this identity of *R,S*-designation arises only because the configuration at C-22 has also been reversed between (47) and (48); a 25*R*-configuration is shown in (51). The wavy lines in (49) denote unspecified or unknown configurations at both C-22 and C-25.

The *R,S* specification may also be affected by substituents attached to ring F or C-26, as in compounds (A) and (B).

* Denotes a trivial name; the systematic name is preferred.



3.4 The name “furostan” is used for the compound of structure (52) (16β, 22-epoxycholestane); this name specifies the configurations at all the asymmetric centres except positions 5, 22, and (if position 26 is substituted) also 25. Configuration at C-5 is designated by use of α or β in the usual way (see Rule 2S-I.5), and configurations at C-22 and, if necessary, C-25 by the sequence-rule procedure, or in all these cases by ξ if unknown.

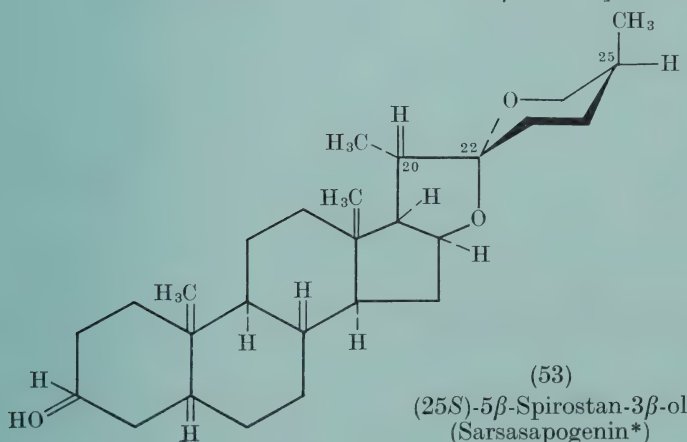


Note

Representative examples of the new standard names and old names* for some common types of spirostan, furostan, and derived structures are given in the annexed Table and formulae.

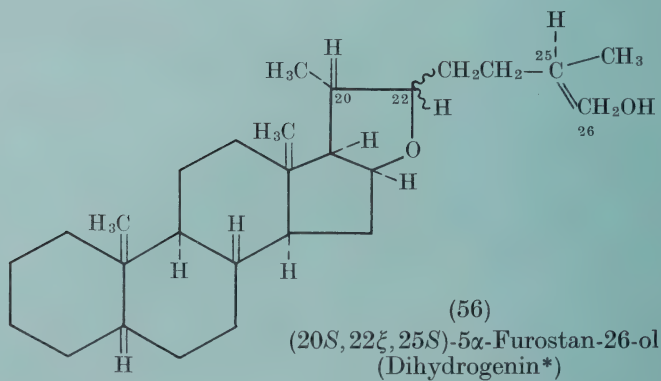
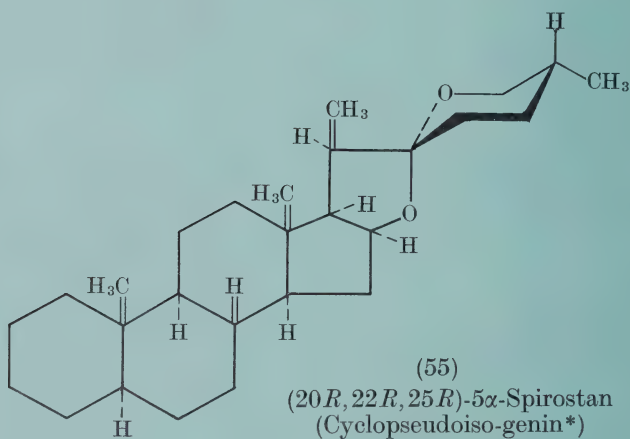
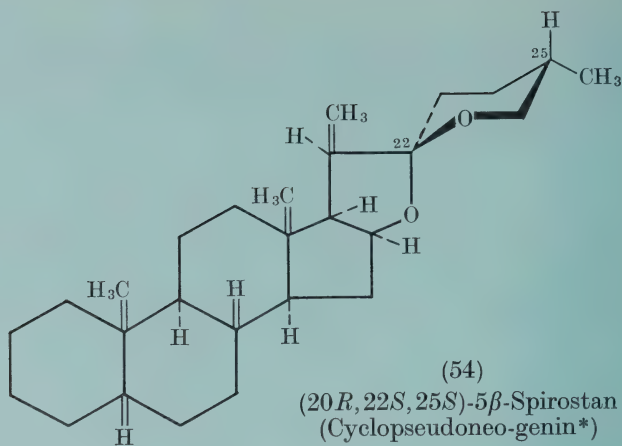
Spirostans and Furostans

Formula type	Standard name	Configurations implied in standard name	Old names (with trivial names for particular compounds in brackets)†
47	25 <i>S</i> -Spirostan	20 <i>S</i> , 22 <i>R</i>	Sapogenin (without prefix) Neo-genin 25- <i>L</i> -genin [Sarsasapogenin is (53)]
51	25 <i>R</i> -Spirostan	20 <i>S</i> , 22 <i>R</i>	Iso-genin 25- <i>D</i> -genin [Smilagenin is (25 <i>R</i>)-5β-Spirostan-3β-ol Tigogenin is (25 <i>R</i> -5α-spirostan-3β-ol]
54	20 <i>R</i> , 22 <i>S</i> , 25 <i>S</i> -Spirostan	—	Cyclopseudoneo-genin (54)
55	20 <i>R</i> , 22 <i>R</i> , 25 <i>R</i> -Spirostan	—	Cyclopseudoiso-genin (55)
56	22 <i>R</i> (or <i>S</i> or ξ), 25 <i>R</i> (or <i>S</i> or ξ)-Furostan	20 <i>S</i>	Dihydrogenin (26-ol) and Dihydropseudogenin (26-ol) [Dihydrosarsasapogenin is 5β, 22ξ, 25 <i>S</i> -furostan-3β, 26-diol Dihydrospeudotigogenin is (58); cf. (57)]
57	25 <i>R</i> (or <i>S</i> or ξ)-Furost-20(22)-en	—	Pseudo-genin [Pseudosarsasapogenin is (59) Pseudosmilagenin is (25 <i>R</i>)-5β-furost-20(22) en-3β, 26-diol]

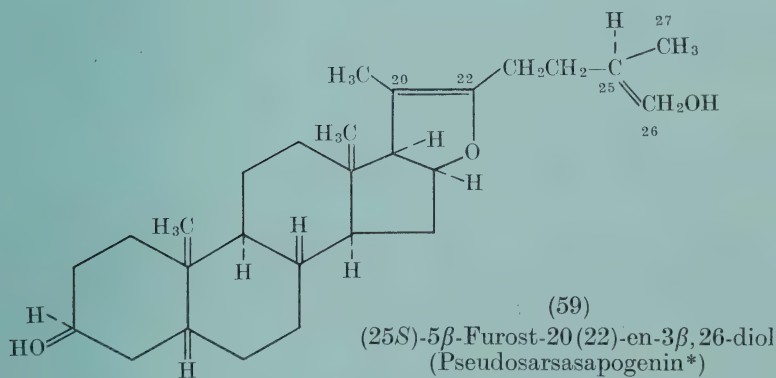
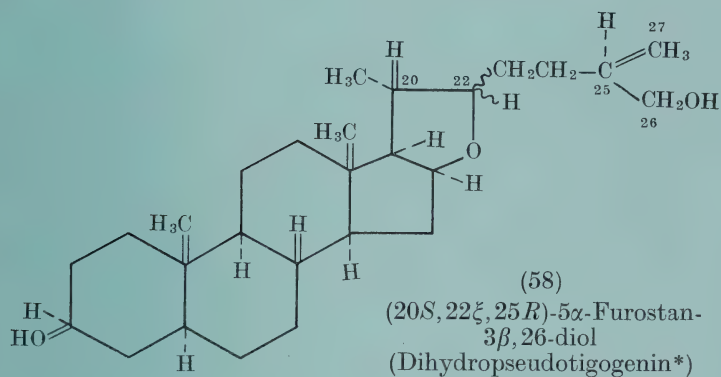
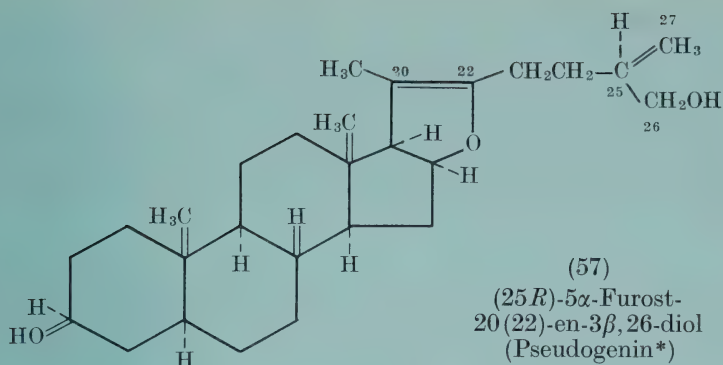


* Standard names are preferred.

† Denotes a trivial name; the standard name is preferred.



* Denotes a trivial name; the standard name is preferred.



* Denotes a trivial name; the standard name is preferred.

Derivatives

Rule 2S-4 (Extended version of Rule S-4)

4.1 Steroid derivatives that can be considered to be formed by modification of, or introduction of substituents into, a parent compound are named by the usual methods of organic chemistry (see IUPAC Nomenclature of Organic Chemistry, Sections A and B (1957) and Section C (1965), Butterworths, London).

Notes

For the benefit of the specialist, those rules of general substitutive nomenclature that apply most often to steroids are outlined here. For full detail the IUPAC Rules cited above should be consulted.

(1) Unsaturation is indicated by changing terminal “-ane” to “-ene”, “-adiene”, “-yne”, etc., or “-an” to “-en”, “-adien”, “-yn”, etc. *E.g.*, 5 α -cholest-6-ene, 5 β -cholesta-7,9(11)-diene, 5-spirosten; see also the names of examples (22)–(25) \diamond .

(2) Most substituents can be designated either as suffixes or as prefixes; a few can be named only as prefixes, the commonest of these being halogens, alkyloxy, alkyl, and nitro groups. When possible, one type of substituent must be designated as suffix. When more than one type is present that could be designated as suffix, one type only may be so expressed and the other types must be designated as prefixes. Choice for suffix is made according to an order of preference that is laid down in the Rules cited above; the most important part of this order, for steroids, is as follows, in decreasing preference: ‘onium salt, acid, lactone, ester, aldehyde, ketone, alcohol, amine, ether. Suffixes are added to the name of the saturated or unsaturated parent system, the terminal “e” of “-ane”, “-ene”, “-yne”, “-adiene”, etc., being elided before a vowel (presence or absence of numerals has no effect on such elisions). The following examples illustrate the use of these principles.

(a) Acids:

Suffix for $-\text{CH}_3 \rightarrow -\text{COOH}$: -oic acid

Suffix for $\text{CH} \rightarrow \text{C}-\text{COOH}$: -carboxylic acid

Examples

11-Oxo-5 α -cholan-24-oic acid

(20S)-3 α -Hydroxy-5-pregnene-20-carboxylic acid

(b) Lactones, other than cardanolides and bufanolides:

The ending “-ic acid” or “-carboxylic acid” of the name of the hydroxy acid is changed to “-lactone” or “-carbrolactone”, respectively, preceded by the locant of the acid group and then the locant of the hydroxyl group, and the prefix “hydroxy” is omitted for the lactonized hydroxyl group.

\diamond For uniformity with the IUPAC Rules cited above, the conventions of *Chemical Abstracts* are used also in the present Rules for the position of locants (positional numerals) and designation of unsaturation. In such matters, and in use of Δ (Greek capital delta) to designate unsaturation (which is not recommended by IUPAC), authors should respect the house customs of the journals to which their papers are submitted.

Examples

3 β -Hydroxy-5 α -cholano-24, 17 α -lactone
(20*R*)-3 β -Hydroxy-5-pregnene 20, 18-carbolactone

(c) Cardanolides and bufanolides:

The -olide ending of these names denotes the lactone grouping, and substituents must be named as prefixes.

(d) Esters of steroid alcohols:

Special procedures are used.

For esters of monohydric steroid alcohols, the steroid hydrocarbon radical name is followed by that of the acyloxy group in its anionic form. The steroid radical name is formed by replacing the terminal "e" of the hydrocarbon name by "yl" and inserting before this the locant and Greek letter, with hyphens, to designate the position and configuration.

Example

5 α -Cholestan-3 β -yl acetate

For esters of polyols the name of the polyol (cf. *g* below) is followed by that of the acyloxy group(s) in its anionic form, with locants when necessary.

Examples

5 β -Cholestane-3 α , 12 α -diol diacetate

5 β -Cholestane-3 α , 12 α -diol 3-acetate 12-benzoate

Estradiol-17 β 17-monoacetate

When an acid, lactone, or spirostan group is also present, the ester group is designated by an acyloxy prefix.

Example

(25*S*)-3 β -Acetoxy-5 β -spirostan

(e) Aldehydes:

Suffixes: -al (denotes change of $-\text{CH}_3$ to $-\text{CHO}$, *i.e.*, without change in the number of carbon atoms)

-aldehyde (denotes change of $-\text{COOH}$ to $-\text{CHO}$, *i.e.*, without change in the number of carbon atoms; name derived from that of the acid)

Prefix: oxo- (denotes change of $>\text{CH}_2$ to $>\text{CO}$, thus also of $-\text{CH}_3$ to $-\text{CHO}$, with no change in the number of carbon atoms)

Examples

5 α -Androstan-19-al

5 α -Cholan-24-aldehyde

19-Oxo-5 α , 17(α H)-etianic acid

Other methods are used for introduction of additional carbon atoms as $-\text{CHO}$ groups.

(f) Ketones:

Suffix: -one

Prefix: oxo-

Examples

5 β -Androstan-3-one

5-Pregnene-3, 20-dione

11-Oxo-5 α -cholan-24-oic acid

(g) Alcohols:

Suffix: -ol

Prefix: hydroxy-

Examples

5 β -Cholestane-3, 11-diol

3 α -Hydroxy-5 α -androstan-17-one

Notes

(1) Composite suffixes -olone and -onol, to denote simultaneous presence of hydroxyl and ketonic groups, are not permitted by IUPAC Rules and should not be used.

(2) A few trivial names exist for hydroxy ketones, such as testosterone for 17 β -hydroxy-4-androsten-3-one (see Rule 2S-4.2).

(h) Amines:

Suffix: -amine

Prefix: amino-

The suffix may be attached to the name of the parent compound or of its radical.

Examples

5-Androsten-3 β -ylamine

or 5-Androsten-3 β -amine

3 β -(Dimethylamino)-5 α -pregnan-20 α -ol

(i) Ethers are named as alkoxy derivatives when another group is present that has priority for citation as suffix.

Examples

3 β -Ethoxycholan-24-oic acid

17 β -Methoxy-4-androsten-3-one

When no such other group is present, ethers of steroid monoalcohols may be named by stating the name of the steroid hydrocarbon radical, followed by the name of the alkyl (or aryl, etc.) radical, and lastly by "ether"; in English these three parts of the name are printed as separate words, for example, 5 α -androsten-3 β -yl methyl ether. For ethers of steroid polyols the same system may be used but with the name of the steroid hydrocarbon radical replaced by the name of the polyol; for partially etherified polyols, locant(s) precede the names of the alkyl (or aryl, etc.) group(s); for example, 5 α -pregnane-3 β , 17 α , 20 α -triol trimethyl ether, 5 α -pregnane-3 β , 17 α , 20 α -triol 3, 17-dimethyl ether, cortisol 21-methyl ether.

4.2 The following are examples of trivial names retained for important steroid derivatives, these being mostly natural compounds of significant biological activity:

Aldosterone 18, 11-Hemiacetal of 11 β , 21-dihydroxy-
20-oxopregn-4-en-18-al

Androsterone 3 α -Hydroxy-5 α -androstan-17-one

Cholecalciferol*	9, 10-Secocholesta-5, 7, 10 (19)-trien-3 β -ol (for seco see Rule 2S-8)
Cholesterol	5-Cholesten-3 β -ol
Cholic acid	3 α , 7 α , 12 α -Trihydroxy-5 β -cholan-24-oic acid
Corticosterone	11 β , 21-Dihydroxy-4-pregnene-3, 20-dione
Cortisol	11 β , 17 α , 21-Trihydroxy-4-pregnene-3, 20-dione
Cortisol acetate	Cortisol 21-acetate
Cortisone	17 α , 21-Dihydroxy-4-pregnene-3, 11, 20-trione
Cortisone acetate	Cortisone 21-acetate
Deoxycorticosterone	21-Hydroxy-4-pregnene-3, 20-dione (<i>i.e.</i> , the 11-deoxy derivative of corticosterone)
Ergocalciferol*	9, 10-Secoergosta-5, 7, 10 (19), 22-tetraen-3 β -ol (for seco see Rule 2S-8)
Ergosterol	5, 7, 22-Ergostatrien-3 β -ol
Estradiol-17 α	1, 3, 5 (10)-Estratriene-3, 17 α -diol
Estradiol-17 β	1, 3, 5 (10)-Estratriene-3, 17 β -diol
Estriol	1, 3, 5 (10)-Estratriene-3, 16 α , 17 β -triol
Estrone	3-Hydroxy-1, 3, 5 (10)-estratrien-17-one
Lanosterol	8, 24-Lanostadien-3 β -ol
Lithocholic acid	3 α -Hydroxy-5 β -cholan-24-oic acid
Progesterone	4-Pregnene-3, 20-dione
Testosterone	17 β -Hydroxy-4-androsten-3-one

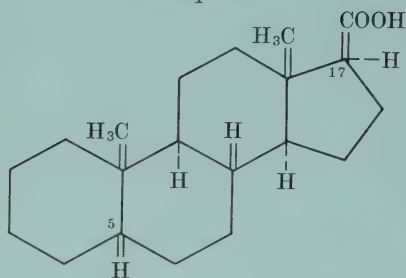
Note

If these trivial names are used as a basis for naming derivatives or stereoisomers, the derived trivial name must make the nature of the modification completely clear and is preferably accompanied at first mention by the full systematic name. For example, in steroid papers "epi" is often used with trivial names to denote inversion at one centre; the name "11-epicortisol" defines the compound fully since cortisol is already defined as the 11 β -alcohol; but the name "epicortisol" does not define the compound and is inadequate.

4.3 Androstane-17-carboxylic acids may be called "etanic acids", although the former (systematic) name is preferred. The orientation of the hydrogen atoms at positions 5 and 17 must in all cases be indicated as 5 α or 5 β , and 17(α H) or 17(β H), respectively.

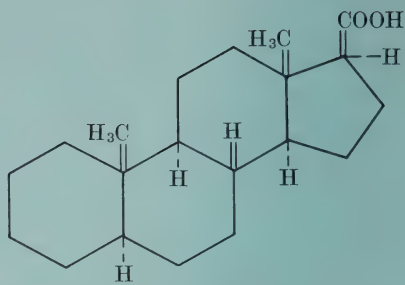
* Included in the List of Trivial Names for Miscellaneous Compounds of Biochemical Importance published by the IUPAC/IUB Commission of Biochemical Nomenclature; see, for example, IUPAC Information Bulletin No. 25, p. 19 (1966); *J. Biol. Chem.* 241, 2987 (1966); *Biochim. Biophys. Acta* 107, 1 (1965).

Examples



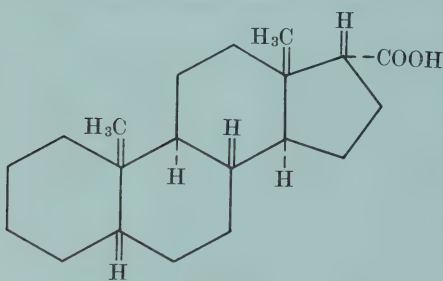
(60)

5β-Androstane-17β-carboxylic
acid (systematic) or
5β,17(αH)-Etianic acid (trivial)



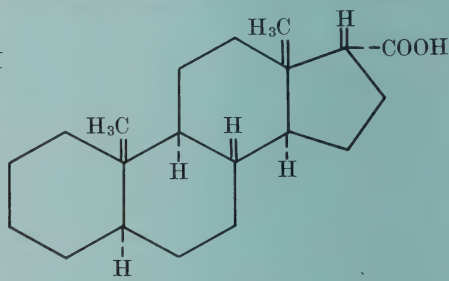
(61)

5α-Androstane-17β-carboxylic
acid (systematic) or
5α,17(αH)-Etianic acid (trivial)



(62)

5β-Androstane-17α-carboxylic
acid (systematic) or
5β,17(βH)-Etianic acid (trivial)



(63)

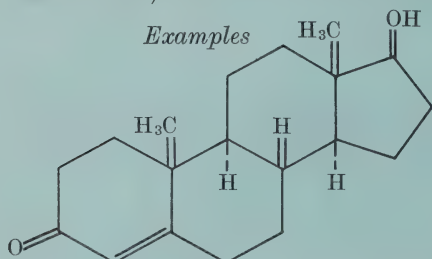
5α-Androstane-17α-carboxylic
acid (systematic) or
5α,17(βH)-Etianic acid (trivial)

Stereochemical modifications

Rule 2S-5 (Extended version of Rule S-5)

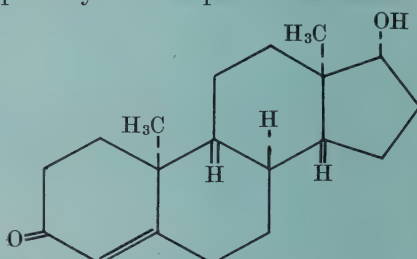
5.1 If, as for instance in a synthetic compound, there is stereochemical inversion at all the asymmetric centres whose configurations do not require to be specified in a name, the italicized prefix *ent*- (a contracted form of *enantio*-) is placed in front of the complete name of the compound. This prefix denotes inversion at all asymmetric centres (including those due to named substituents) whether these are cited separately or are implied in the name.

Examples



(64)

17β-Hydroxy-4-androsten-3-one
(Testosterone)



(65)

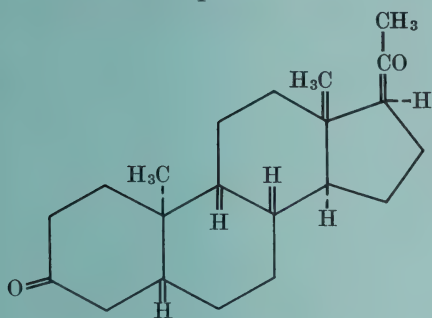
ent-17β-Hydroxy-4-androsten-
3-one
(*ent*-Testosterone)

Note

When Roman or Arabic numerals are used to enumerate formulae, the prefix *ent* may be used to indicate the enantiomer. Thus, *e.g.* (65) above may be designated (*ent*-64).

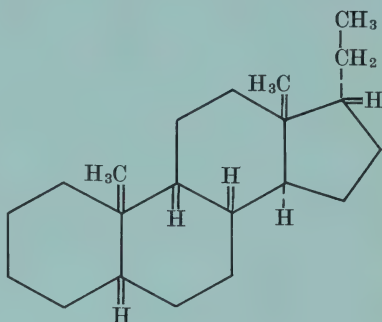
5.2 If there is stereochemical inversion at a minority of the asymmetric centres whose configurations do not require to be specified in a name, the configuration of the hydrogen atoms or substituents at the affected bridge-heads, or the carbon chain (if any) at position 17, are stated by means of a prefix or prefixes α or β , each with its appropriate positional numeral, placed before the stem name laid down in the preceding Rules.

Examples



(66)

5 β ,9 β ,10 α -Pregnane-3,20-dione



(67)

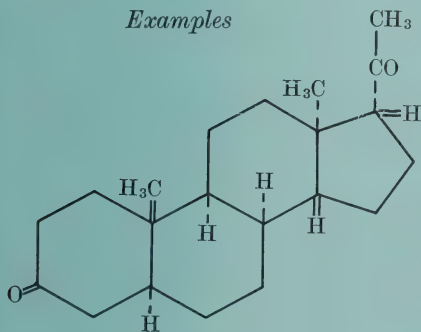
5 β ,9 β ,17 α -Pregnane

5.3 The enantiomer of a compound designated as in Rule 5.2 is given the same name preceded by *ent*-.

Note

This Rule covers the compounds in which there is inversion at a majority, but not all, of the asymmetric centres that do not require to be specified in the name.

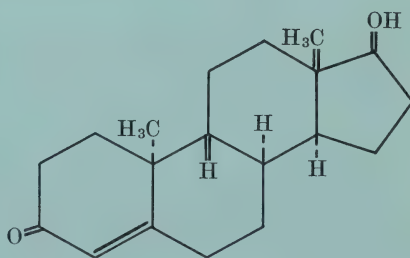
Examples



(68) = (*ent*-66)

ent-5 β ,9 β ,10 α -Pregnane-3,20-dione

(Not 5 α ,8 α ,13 α ,14 β ,17 α -Pregnane-3,20-dione^a)



(69)

ent-17 α -Hydroxy-13 α ,14 β -androstan-3-one

(Not 17 β -Hydroxy-8 α ,9 β ,10 α -androstan-3-one)

5.4 If there is stereochemical inversion at half of the asymmetric centres whose configurations are implied in the stem name of a "normal" steroid (*e.g.*, 70), the prefixes to be specified in the name of the stereoisomer are that set which includes the number occurring first in the series 8, 9, 10, 13, 14, 17 without or with the prefix *ent* as appropriate.

		Configuration at asymmetric centres	Name
(70) "Normal" steroid		$8\beta, 9\alpha, 10\beta, 13\beta$	Androsta- 5, 14-diene
(71) Steroid inverted at 8 and 10; "normal" at 9 and 13		$8\alpha, 9\alpha, 10\alpha, 13\beta$	$8\alpha, 10\alpha$ - Androsta- 5, 14-diene
(72) (<i>ent</i> -71) Steroid inverted at 9 and 13; "normal" at 8 and 10		$8\beta, 9\beta, 10\beta, 13\alpha$	<i>ent</i> - $8\alpha, 10\alpha$ - Androsta- 5, 14-diene

Note

(72) could also logically be named " $9\beta, 13\alpha$ -Androsta-5, 14-diene"; this name might seem simpler, but it has the disadvantage that it does not indicate that (72) is the enantiomer of (71).

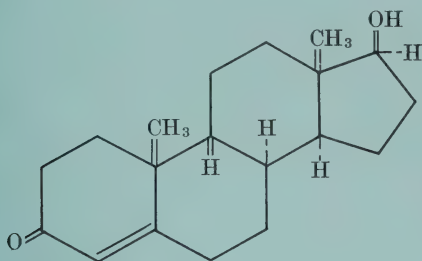
5.5 Racemates, as for instance obtained by synthesis, are named by use of an italicized prefix *rac*- (an abbreviation of *racemo*-), placed before the complete name of the compound, the enantiomer chosen for naming being that required by Rules 2S-5.1 to 2S-5.4.

Example

A racemate composed of (64) and (65) (= *ent*-64) is named:
rac-17 β -Hydroxy-4-androsten-3-one
or *rac*-Testosterone

5.6 (a) When the relative, but not the absolute, configuration of two or more asymmetric centres in a steroid derivative is known, as for instance for a compound obtained by synthesis, the 10β -configuration is taken as basis for the name; or, if C-10 is not asymmetric or is absent, the lowest-numbered asymmetric bridgehead is designated α (or R); the other asymmetric centres are then considered as α or β (or R or S) relative to that one; and the whole name is prefixed by *rel*- (italicized). Individual asymmetric centres may be referred to as α^* , β^* , R^* , or S^* (spoken, alpha star, R star, etc.) but these symbols are not used in the name of the compound.

(b) When both enantiomers of known relative, but unknown absolute, configuration are prepared, they are distinguished by a prefix (+)-*rel*- or (–)-*rel*-, where the plus or minus sign refers to the direction of rotation of plane-polarized light (the wavelength, solvent, temperature and/or concentration must be added when known to affect this sign).

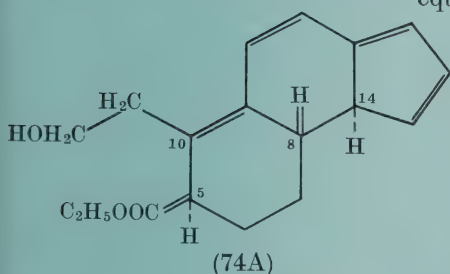


(73)

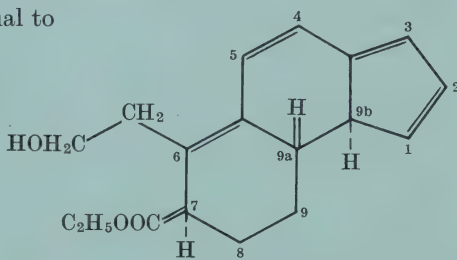
The dextrorotatory form having either this or the enantiomeric configuration would be named:

(+)-*rel*-17β-Hydroxy-8α,9β-androst-4-en-3-one

equal to



(74A)



(74B)

(74A) *rel*-(Ethyl 2-hydroxy-2,3-seco-*A*-nor-5α-gona-9,11,13(17),15-tetraen-3-oate

(for seco see Rule 2S-8 and for nor see Rule 2S-7)

or (74B) *rel*-[(7*R*,9*aS*,9*bS*)-Ethyl 8,9,9*a*,9*b*-tetrahydro-7*H*-benz[*e*]indene-7-carboxylate

Note

At some stage in synthetic work on steroids, names of intermediates have to be changed from a system used in general organic chemistry to the steroid system. The names (74A) and (74B) illustrate such a change and it should

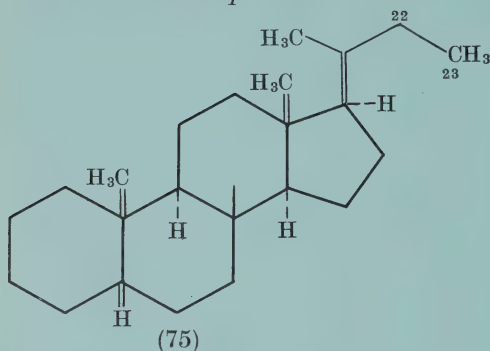
be noted (i) that not merely the name but also the numbering are usually changed and (ii) that the steroid name usually avoids the need to specify the configuration at each asymmetric centre. The latter factor will often indicate at what point in a synthesis the change of nomenclature is desirable.

Shortening of sidechains and elimination of methyl groups

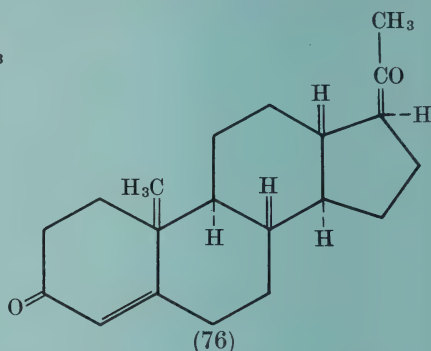
Rule 2S-6 (Expanded from Rule S-6)

6.1 Elimination of a methylene group from a steroid sidechain (including a methyl group) is indicated by the prefix "nor"-, which in all cases is preceded by the number of the carbon atom that disappears. When alternatives are possible, the number attached to nor is the highest permissible. Elimination of two methylene groups is indicated by the prefix "dinor-".

Examples



24-Nor-5 β -cholane



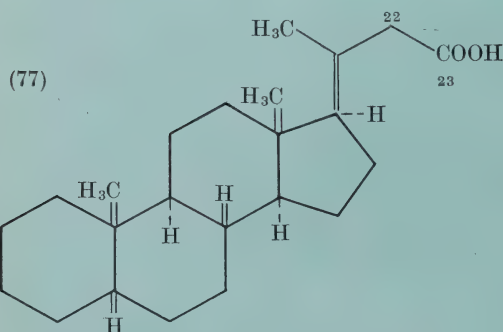
18-Nor-4-pregnene-3,20-dione

Exceptions

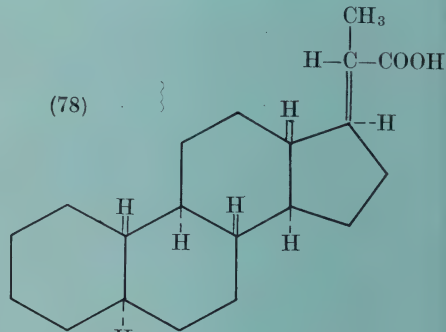
By Rules 2S-2.1 and 2S-2.2 the names gonane (for 18,19-dinorandrostane) and estrane (for 19-norandrostane) constitute exceptions to the above Rule 2S-6.1. The names gonane and estrane are used also as parent names for their derivatives.

However, 18-nor- and 19-nor- are used with other trivial names, as in 19-norpregnane, 18,19-dinorspirostan, 18-norestrone.

The compound produced by shortening the 17-sidechain of pregnane is named 17-methylandrostanene rather than 21-norpregnane. See also Note to Rule 2S-2.2.



24-Nor-5 β -cholan-23-oic acid



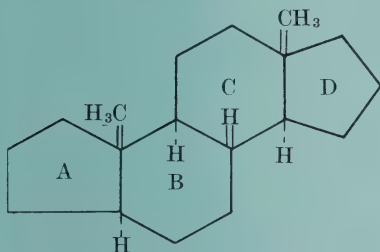
18,19-Dinor-5 α -pregnane-20 α -carboxylic acid

Ring contraction or expansion

Rule 2S-7 (Amended version of Rule S-7)

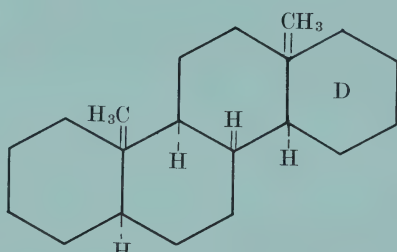
7.1 Ring contraction and ring expansion (other than insertion of atoms between directly linked bridgeheads or, when a steroid sidechain is present, between C-13 and C-17) is indicated by prefixes “nor” and “homo”, respectively, preceded by an italic letter indicating the ring affected. For loss or insertion of two methylene groups, “dinor” and “dihomo” are used. “Homo” and “nor”, when occurring in the same name, are cited in alphabetical order*.

Examples



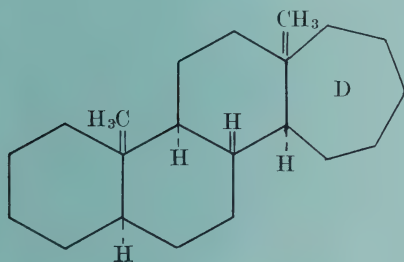
(77)

A-Nor-5 α -androstane



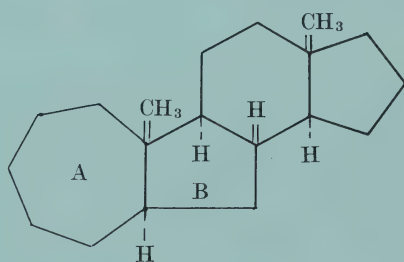
(78)

D-Homo-5 α -androstane



(80)

D-Dihomo-5 α -androstane



(81)

A-Homo-B-nor-5 α -androstane

Notes

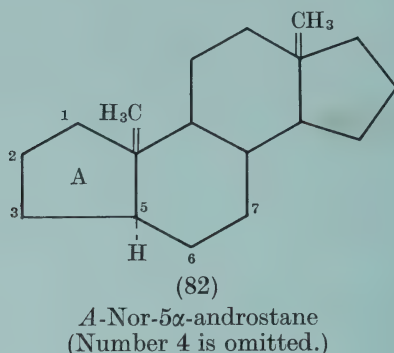
(1) By too extended use, this nomenclature can be applied to compounds whose steroid character is excessively modified. It is recommended that it be confined to steroids containing at least one angular methyl group, or a steroid 17-sidechain, or a steroidal group on ring *D* (e.g., a spirostan); also that no more than two of the steroid rings may be altered by any combination of the operations denoted by “nor” and “homo”. When these conditions are not met, general systematic nomenclature should be used.

(2) Names incorporating “homo” and “nor” are normally preferred to alternatives incorporating “cyclo” and “seco” [cf. example (86)].

* Alphabetical order is used for any combination of cyclo, homo, nor, and seco; they are placed immediately before the stem name and after any prefixes denoting substituents.

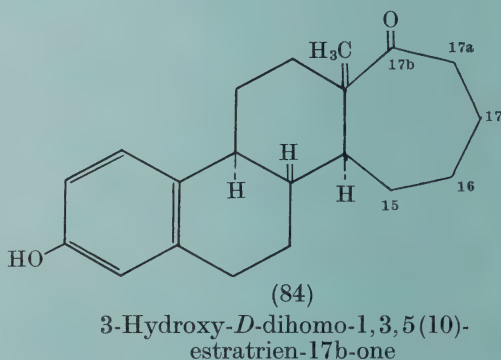
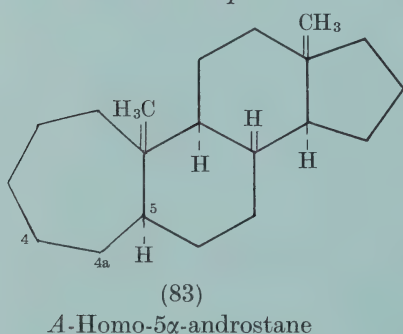
7.2 On ring contraction the original steroid numbering is retained, and only the highest number(s) of the contracted ring, exclusive of ring junctions, is deleted.

Example



7.3 On ring expansion (other than insertion of atoms between directly linked bridgeheads or, when a 17-sidechain is present, between C-13 and C-17), the letter a (and b, etc., as necessary) is added to the highest number in the ring enlarged exclusive of ring junctions, and this letter and number are assigned to the last peripheral carbon atom in the order of numbering of the ring affected.

Examples



7.4 Ring expansion by formal insertion of a methylene group between directly linked bridgeheads is indicated as shown in the annexed Table. The italic capital letters denote the ring(s) affected; the locants in parentheses (which are included in the name) are those of the inserted methylene groups.

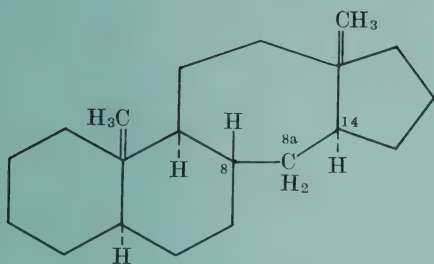
CH₂ added between

C-5 and C-10
C-8 and C-9
C-8 and C-14
C-9 and C-10
C-13 and C-14

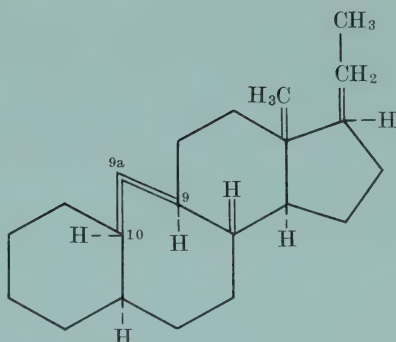
Prefix used

AB(10a)-Homo
BC(8a)-Homo
C(14a)-Homo
B(9a)-Homo
CD(13a)-Homo

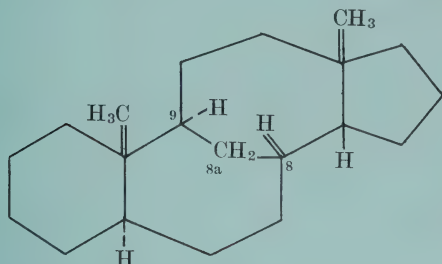
Examples



(85) *C(14a)*-Homo-5 α -androstane

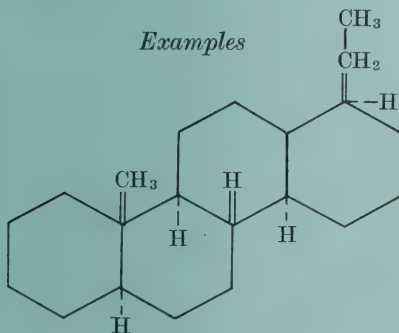


(86) *B(9a)*-Homo-19-nor-5 α ,10 α (H)-pregnane*

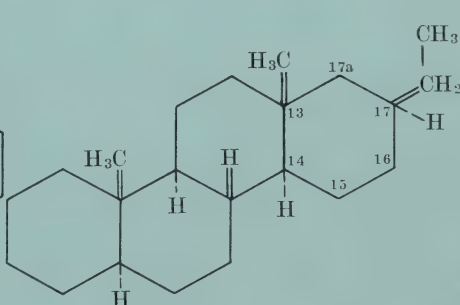


(87) *BC(8a)*-Homo-5 α -androstane

7.5 Expansion of ring *D* by insertion of atoms between C-13 and C-17: The names “*D*-homopregnane”, “*D*-homocholane”, etc., are used only for the isomer with the sidechain at position 17a [cf. example (88)]. Isomers with the sidechain at position 17 (formed by formal insertion of a methylene group between C-13 and C-17) are named as derivatives of androstane, estrane, or gonane [cf. example (89)]. As exceptions, furostans and spirostans into which a methylene group has been formally inserted between C-13 and C-17 are given these names with an added prefix “*D*(17a)-homo” [cf. example (90)].

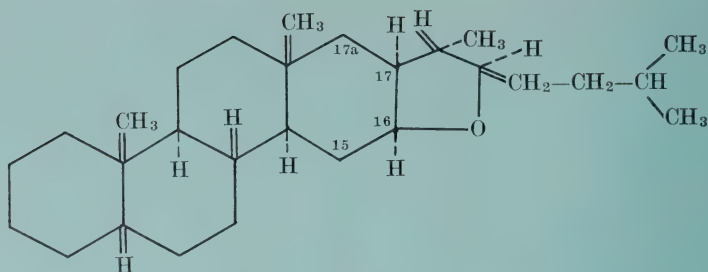


(88) *D*-Homo-5 α -pregnane



(89) 17 β -Ethyl-*D*(17a)homo-5 α -androstane

*This name is preferred to 9 β ,19-cyclo-9,10-seco-5 α ,10(α H)-pregnane (see Note 2 to Rule 2S-7.1). This skeleton is contained in some *Buxus* alkaloids.



(90)

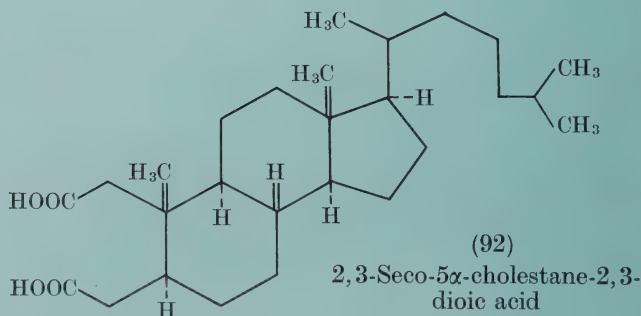
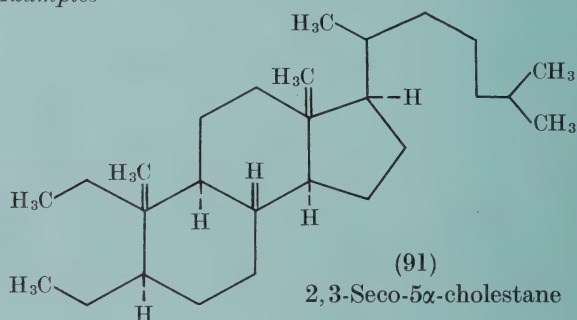
(22*R*)-*D*(17*a*)-Homo-5β-furostan

Ring fission

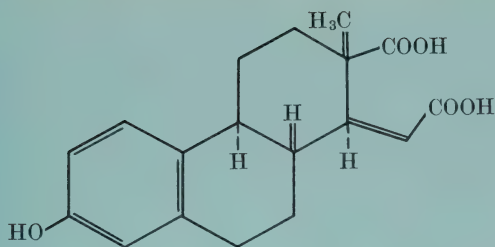
Rule 2S-8 (Unchanged from Rule S-7.4)

8.1 Fission of a ring, with addition of a hydrogen atom at each terminal group thus created, is indicated by the prefix "seco-", the original steroid numbering being retained*.

Examples

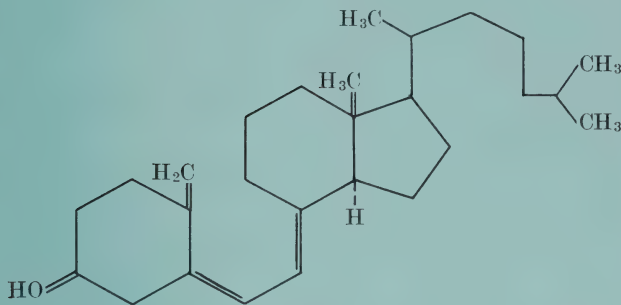


*If more than one ring is opened, general systematic nomenclature may be preferable. The principles of Note 1 to Rule 2S-7.1 apply also to seco-steroids.



(93)

3-Hydroxy-16,17-seco-1,3,5(10)-
estratriene-16,17-dioic acid



(94)

9,10-Seco-5,7,10(19)-cholestatrien-3 β -ol
(trivial name: cholecalciferol*)

Modification by bond migration (abeo system)

Rule 2S-9 (New)

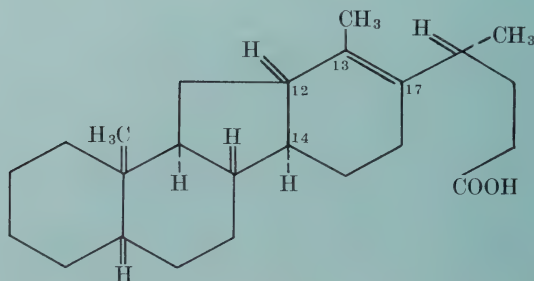
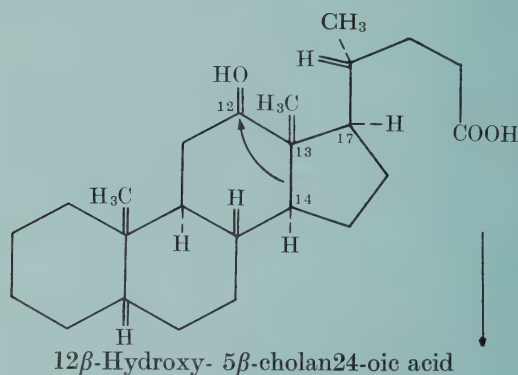
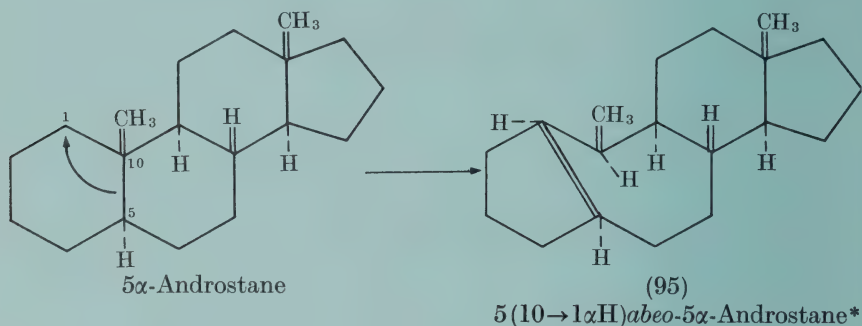
9.1 A compound that does not possess a steroid skeleton but may be considered formally to arise from a steroid by bond migration may be given the name laid down in the preceding Rules for the steroid in question, to which is attached a prefix of the form $x(y \rightarrow z)$ abeo-. This prefix is compiled as follows: A numeral denoting the stationary (unchanged) end of the migrating bond (x) is followed by parentheses enclosing (i) the number denoting the original position (y) from which the other end of this bond has migrated, (ii) an arrow, and (iii) the number (z) denoting the new position to which the bond has moved. The closing parenthesis is followed by *abeo-* (Latin, I go away) (italicized) to indicate bond migration. The original steroid numbering is retained for the new compound and is used for the numbers x , y , and z . Such of the customary letters as are necessary are added to specify the resulting stereochemistry.

* This trivial name is retained (see Rule 2S-4.2).

Note

The *abeo* nomenclature described in this Rule is permissive, not compulsory. It is most suitable for use in discussions of reaction mechanism and biogenesis. For registration in a general (non-steroid) compendium the general systematic names may be preferable, particularly when names of steroid type can be conveniently assigned by the homo-nor method. Differences in numbering between *abeo* names and other systematic names should be particularly noted [cf. example (96)].

Examples



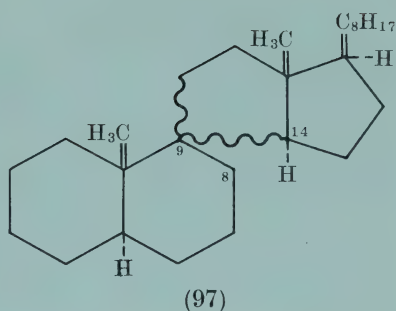
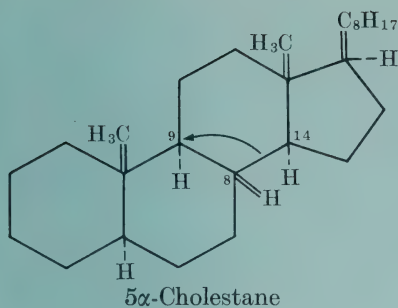
(96) 14(13→12βH)*abeo*-5β-Chol-13(17)-en-24-oic acid[‡]

*Name according to Rule 2S.7.4:

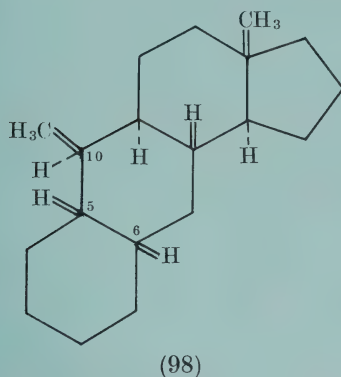
9aβ-Methyl-*B*(9a)-homo-*A*-nor-1αH,5α-estrane.

‡ Name according to Rules 2S.2.4 and 2S.8.1:

12α,14β-Cyclo-13,14-seco-5β-chol-13(17)-en-24-oic acid.



14(8→9 ξ)abeo-5 α -Cholestane*



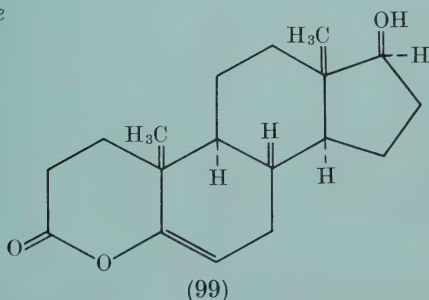
1(10→6 β)abeo-5 β -Androstane (An anthrasteroid)

Hetero modifications

Rule 2S-10 (Unchanged from Rule S-7.5)

10.1 If hetero atoms occur in the ring system of a steroid the replacement ("oxa-aza") system of nomenclature is used with steroid names and numbering (cf. IUPAC Rule B-4; also Introduction to IUPAC Rules C-0.6).

Example



17 β -Hydroxy-4-oxaandrost-5-en-3-one

* The configuration at C-9, if known, is assigned by the sequence-rule procedure (ref.1).

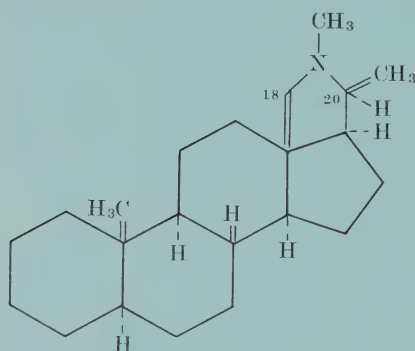
Steroid alkaloids

Rule 2S-11 (New)

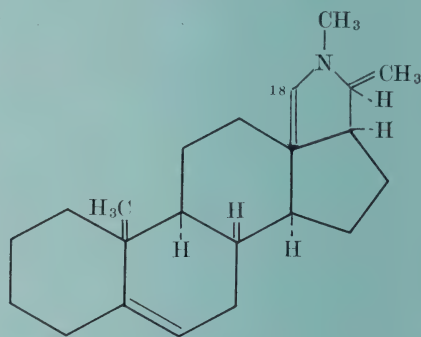
11.1 When readily possible, systematic names for steroid alkaloids are derived from pregnane or some other steroid parent name. Trivial names for other steroid alkaloids are chosen so that the name for the saturated system ends in “-anine”. In names for unsaturated compounds this ending is changed to “-enine”, “-adienine”, etc., as appropriate. When asymmetry exists at positions 8, 9, 10, 13, 14, 16, 17, 20, or 23, it is implied in the name, as set out in the annexed Table and formulae, and divergences are designated as laid down in Rule 2S-5. Configurations at positions 5, 22, and 25 must be specified with the name. Sequence-rule symbols are used for positions numbered 20 or higher.

Examples

Typical examples of parent names for groups of alkaloids are given in the annexed Table and the corresponding formulae. It must be noted that substitution or unsaturation may alter the *R,S* designations for derivatives.



(100)
5 α -Conanine*



(101)
5-Conenine*

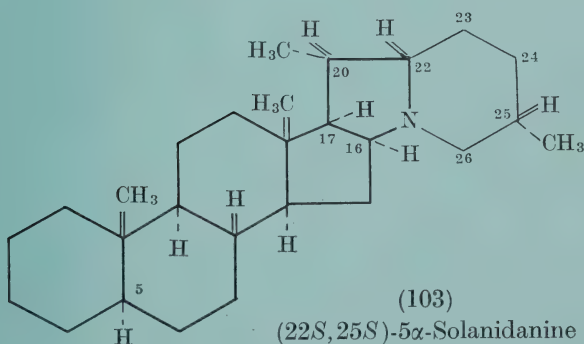
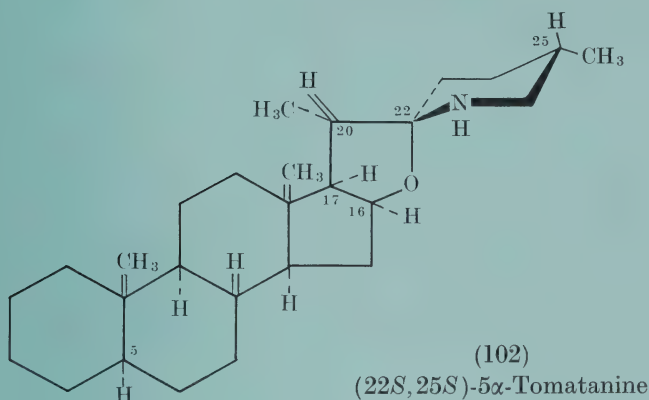
Parent names for groups of steroid alkaloids (a)

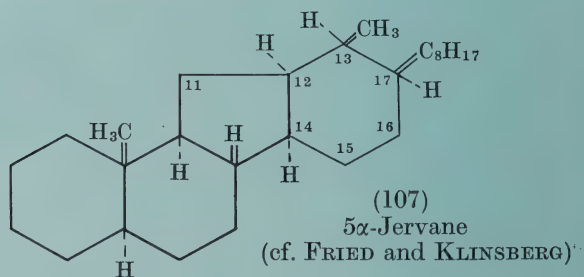
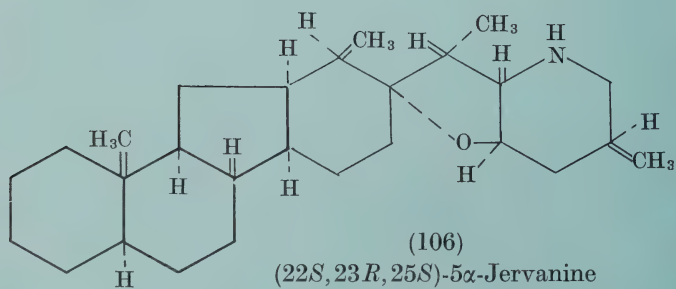
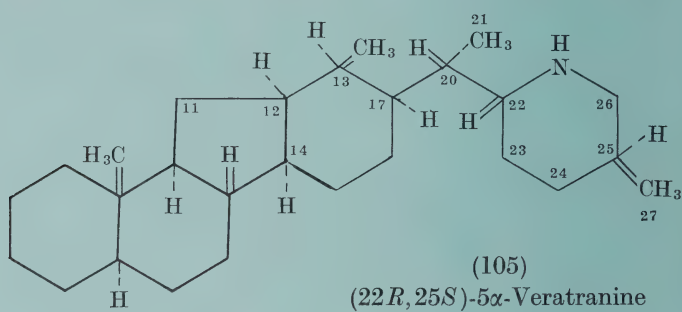
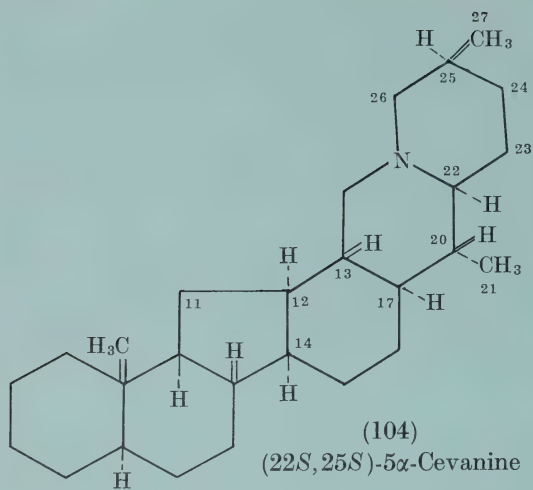
Formula	Name of parent	Stereochemistry (b) implied in the name, as shown in the formula	Stereochemistry to be indicated by sequence-rule prefixes (or ξ)
100	Conanine	17 α H, 20S	—
102	Tomatanine (c)	16 α H, 17 α H, 20S	22, 25
103	Solanidanine (d)	16 α H, 17 α H, 20S	22, 25
104	Cevanine (e)	17 α H, 17 α H, 20R	22, 25
105	Veratranine (e, f)	17 α H, 20S	22, 25
106	Jervanine (e, f)	17 α O, 20R	22, 23, 25

(a) Some of the names in this Table were suggested in the Introduction to “Optical Rotatory Power, 1a, Steroids”, Tables des Constantes, Pergamon Press, Oxford, 1965, pp.2a and 2f.

* Cf. R. D. HAWORTH and M. MICHAEL: *J.Chem.Soc.* 1957, 4973.

- (b) Additional to that at positions 8, 9, 10, 13, and 14.
- (c) The compounds are oxa-aza analogues of the spirostans (which are dioxo spiro compounds). Formulae are conveniently drawn analogously to those of the spirostans.
- (d) This group includes rubijervine and isorubijervine.
- (e) These structures contain a *D*-homo-*C*-nor skeleton, with the stereochemistry shown. However, they are commonly considered as 14(13→12) *abeo* structures and are numbered as such.
- (f) Jervanine, as defined here, is the same as veratranine except for addition of an epoxy bridge, but it is convenient to have two separate names: the veratranine skeleton (see 105) is present in the alkaloid veratramine. It should be noted that the name 5 α -jervane has been used for the rearranged hydrocarbon skeleton (107) [J. FRIED and A. KLINGSBERG: *J. Amer. Chem. Soc.* 75, 4934 (1953)], for which the *abeo*-type numbering given in (107) is here recommended.





APPENDIX

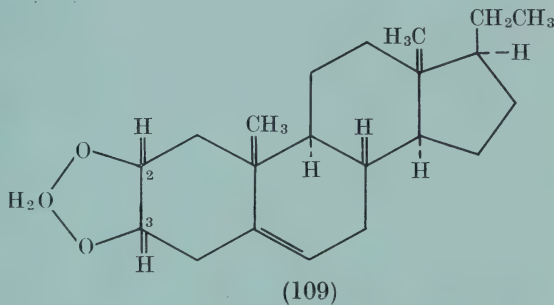
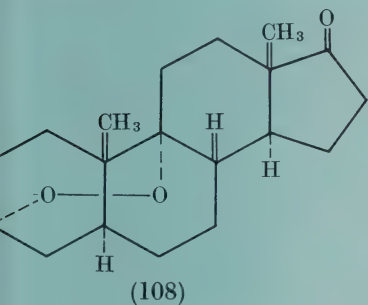
Guide lines for steroids containing additional rings

1. General

When additional rings are formed within, or on, a steroid nucleus, situations often arise where either the resemblance to a normal steroid is obscured or the steroid-type name becomes so complex that recourse to general systematic nomenclature is preferable. On the other hand, the general rules, with one exception, are based on that form of each component which contains the maximum number of conjugated double bonds, the whole fused system is then renumbered, and the stereochemistry must be defined separately for each chiral position; the final name resulting is then cumbersome and in a form that is often barely recognizable by a steroid specialist chemist and even less so by a biochemist or biologist. The paragraphs below give suggestions as to how general nomenclature may be modified to incorporate steroid names, but without an attempt to legislate rigidly or to cover every case. The decision whether any one compound shall receive such a modified steroid name or a general systematic name is left to authors and editors in the particular circumstances of each case. Nor are the requirements of journals and compendia or abstracts necessarily identical.

2. Rings derived from functional groups

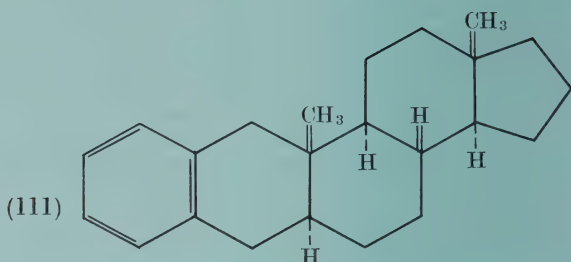
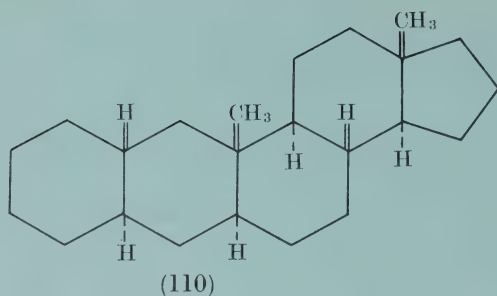
Bivalent functional groups such as -O- and -O-O- linked to two different positions, thus forming additional rings, are named by the ordinary methods of organic chemistry; for example (108) is $3\alpha,9$ -epidioxy- 5α -androstan-17-one. Similarly, methylenedioxy derivatives are best named as such, *e.g.* (109) $2\beta,3\beta$ -methylenedioxy-5-pregnene. In the same way, lactones and acetals formed by linkage between two different positions of a steroid skeleton are best named as such instead of framing the name on the newly modified ring system.



3. Additional carbocyclic or heterocyclic fused rings

It is tempting to adapt the simple substitutive procedure for fusion of steroid nuclei with simple carbocyclic rings, particularly if the latter are saturated. Thus (110) might be named $2\alpha,3\beta$ -tetramethylene- 5α -androstan-17-one*. However, formation of additional rings by alkylene ($-\text{[CH}_2\text{]}_x-$) prefixes is not in accord with IUPAC nomenclature and is often difficult to apply when unsaturation is present. Alternatives are thus preferable.

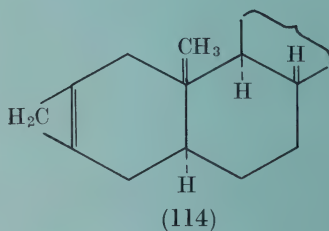
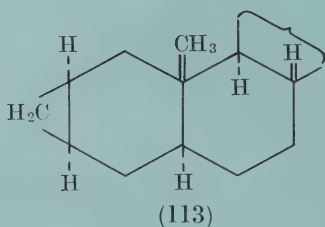
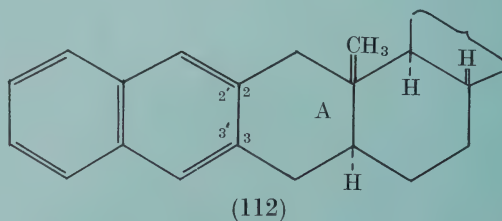
* For simplicity, nomenclature in this Appendix is mostly described in terms of androstane, and partial formulae are to be understood accordingly. The principles, however, are general.



The exceptional case (Rule A-23.5) referred to above enables 2,3-benz-5 α -androst-2-ene to be a name for (111), and a slight extension of the rule would allow (110) to be called 1 α ,2 β -cyclohexano-5 α -androstane. Such methods might be used in simple cases but these too become difficult when complex ring systems are fused and often when unsaturation is present in the additional component.

For a general procedure it is better to modify systematic IUPAC general practice to permit the steroid component to be cited in a reduced state, the reason why modification is necessary at all being of course the wish to keep the description of the stereochemistry as simple as possible. The suggestions below are closely similar to present practices of *Chemical Abstracts*.

An additional carbocyclic component is cited in its most unsaturated form by its fusion name (usually ending in -o), placed in front of the name of the steroid component, and the position of fusion is indicated by numerals in

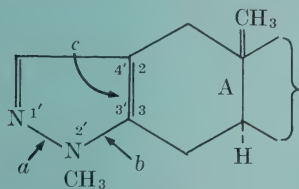


square brackets; for instance, benz[2,3]-5 α -androstene for (111). Here note that the unsaturation of the benzo ring causes unsaturation also in the steroid component and this must be cited (-2-ene). Similarly (112) is naphtha[2',3':2,3]-5 β -androst-2-ene; the steroid A ring is still considered unsaturated even though it may be preferred to write the naphthalene double bonds as in the formula shown; note also that the locants for the non-steroid component receive primes, and that, when choice is possible, its locants for ring fusion are as low as possible and in the same direction as in the steroid component (*i.e.*, not 6',7':2,3 or 3',2':2,3).

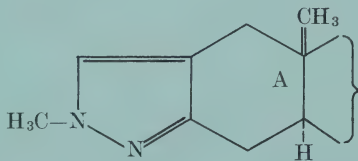
The reduced compound (110) is then 2 β ,3 α ,3',4',5',6'-hexahydrobenz[2,3]-5 α -androstane. Note the citation of the configuration at the new ring junction positions and that the steroid component is now cited in its saturated state.

Two further points can be illustrated with (113). Consider first the hydrocarbon where X = H. The additional ring is cited as cyclopropa, denoting an unsaturated three-membered ring as in (114). In (114) the position of the "extra" (indicated) hydrogen must be cited as 2'*H*. Reduction of (114) to (113; X = H) adds 2 α ,3 α -dihydro to the name, which thus becomes 2 α ,3 α -dihydro-2'*H*-cyclopropa[2,3]-5 α -androstane. If X were not hydrogen but, say, OH, the hydro prefixes would still be needed to show the state of hydrogenation and the OH group would be named additionally; in such cases it is preferable to state the configuration for the OH group that is present rather than that of the H atom that has been replaced; the name then becomes 2 α ,3-dihydro-2'*H*-cyclopropa-[2,3]-5 α -androstane-3 α -ol.

The same fundamental principle can be used for heterocyclic components, but conveniently modified to accord with general nomenclature as follows: (a) the heterocyclic component is cited after the steroid component (to permit modification of the ending for salt-formation, etc.), and (b) the position of fusion of the heterocyclic component is cited by letters as in the standard IUPAC and Ring Index method. Thus, (115) is 2'-methyl-2'*H*-5 α -androst-2-eno[3,2-*c*]pyrazole; note the numbering of the pyrazole ring so that numbers for ring fusion are as low as possible; if the methyl group in (115) were replaced by hydrogen, the double bonds would be placed in the mesomeric pyrazole ring just as in (115) so as to retain this low numbering for ring fusion. In the isomer (116) the steroid component is no longer unsaturated and is therefore cited as androstano-; the full name for (116) is 1'-methyl-1'*H*-5 α -androstano[3,2-*c*]pyrazole.

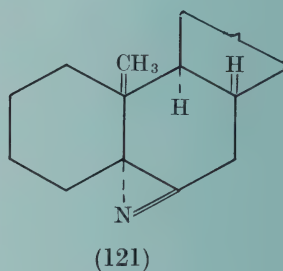
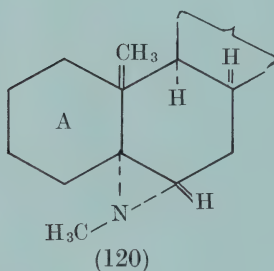
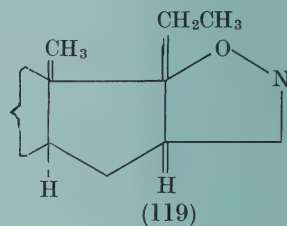
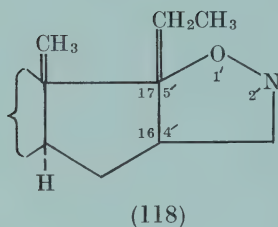
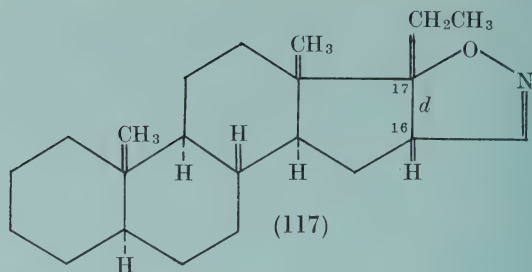


(115)



(116)

Further problems arise when ring fusion involves a quaternary carbon atom. The name for (117), for instance, could be built up as follows: to 5 α -pregnane is fused an isoxazole *skeleton*, giving (118); into this, only one double bond can be introduced, so that one hydrogen atom must be added as indicated hydrogen, which gives a 4' β *H*- prefix and a skeleton (119). The last step, inserting the double bond, gives the full name 4' β *H*-5 α -pregnano[16,17-*d*]isoxazole, even though it appears in (117) as if the heterocyclic ring should be named as the partly hydrogenated system pyrazoline.



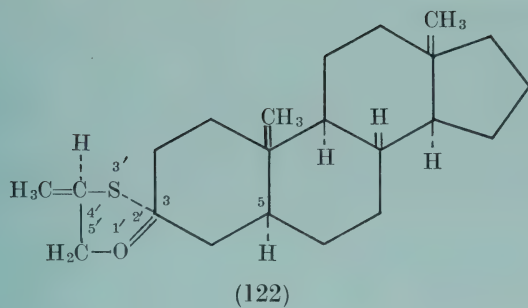
Not all such fusions cause all these complications. For instance, for (120) one fuses androstane to azirine, obtaining a skeleton into which one inserts a double bond as in the hypothetical compound (121); then, clearly, (120) is 1',3'-dihydro-1'-methyl-5 α -androstano[5,6-*b*]azirine.

4. Stereochemistry

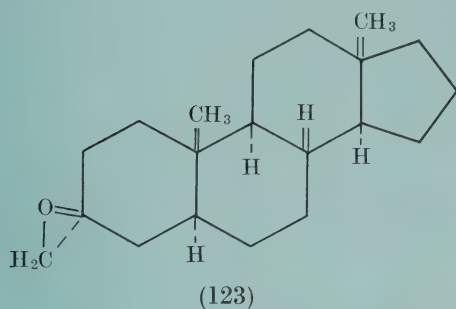
Stereochemistry in additional rings that lie in the approximate plane of rings A-D is cited as α or β , but in other cases by means of sequence-rule symbols.

5. Spiro derivatives

Spiro derivatives of steroids are named in accordance with the principles laid down in IUPAC Rules A-41, A-42, B-10, and B-11. Additional stereochemistry due to the spiro junction and substituents in the non-steroid ring is designated by the sequence-rule procedure. Alternative names permitted by IUPAC Rules are illustrated for (122) and (123).



4' *R*-Methyl-*R*-spiro[5 α -androstande-3,2'-(1',3'-oxathiolane)]
or 5 α -Androstande-3 *R*-spiro-2'-(4' *R*-methyl-1',3'-oxathiolane)



(3*S*)-Spiro[5 α -androstande-3,2'-oxiran]-17 β -ol
or (3*S*)-5 α -Androstande-3-spiro-2'-oxiran-17 β -ol

TENTATIVE PROPOSALS FOR NOMENCLATURE* OF ABSOLUTE CONFIGURATIONS CONCERNED WITH SIX-COORDINATED COMPLEXES BASED ON THE OCTAHEDRON**

1. Introduction

1.1 Configuration

For spectroscopic purposes and for following the stereochemical course of substitution reactions it is of interest to consider, for example, tris- and bis-bidentate six-coordinated complexes based on the octahedron as related through the configurations depicted in Fig.1 (a) and (b). Here the edges spanned by the chelate rings are drawn as heavy lines. The chelate rings are thought of as devoid of chemical significance in the sense that the chelating ligands may be identical or different, and may be symmetrical or not. Similarly the two X's represent two monodentate ligands which may or may not be identical. It is desired, in all generality, to have a designation of chirality which is independent of the chemical nature of the chelating ligands and which only depends on the relative positions of the heavy line edges which represent the bidentate ligands or the bidentate units of polydentate ligands.

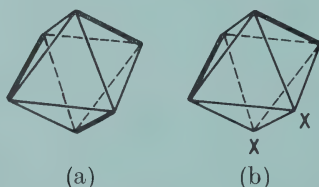


Fig. 1 General "octahedral" systems containing three (a) and two (b) bidentate ligands represented by the edges (drawn as heavy lines) which they span. It is desired to characterize these systems as having the same absolute configuration independently of their chemical significance. They have both been designated by Δ in the present proposal

1.2 Conformation

Further for spectroscopic purposes it is of interest to designate the conformation of chelate rings relative to the central atom or ion, but independently of the other atoms forming the chelate ring and also of the substituents of these atoms.

* The rules proposed here are given in short form in paragraph 8 and 9 of this communication

** Comments should be sent to the chairman of the Commission, Prof. K.A.JENSEN, Chemical Laboratory II of the University of Copenhagen, The H.C.Ørsted Institute, Universitetsparken 5, 2100 Copenhagen Ø

1.3 *The present proposals*

All the tentative rules which follow are based on the fact that two skew and non-orthogonal lines define a helical system. They primarily describe a nomenclature for the absolute configuration of classes comprising *cis*-bis-bidentate and tris-bidentate complexes and the absolute conformation of five-membered chelate rings. However, since the rules are based on general grounds, they lend themselves readily to application to more complicated situations, *i.e.* polydentate chelate systems and larger chelate rings.

In the chemical literature there exist different proposals for the nomenclature of the systems, devoid of chemical significance, which are under consideration here. These proposals are generally based upon helicities about symmetry or pseudo-symmetry axes. The present proposals are independent of symmetry concepts and thereby easier to generalize to situations where symmetry is absent.

2. **Basic principle**

Two skew lines which are not orthogonal to each other make up a helical system as illustrated in Fig. 2 and 3. Two skew lines possess the property of having one and only one normal in common. In Fig. 2 one of the skew

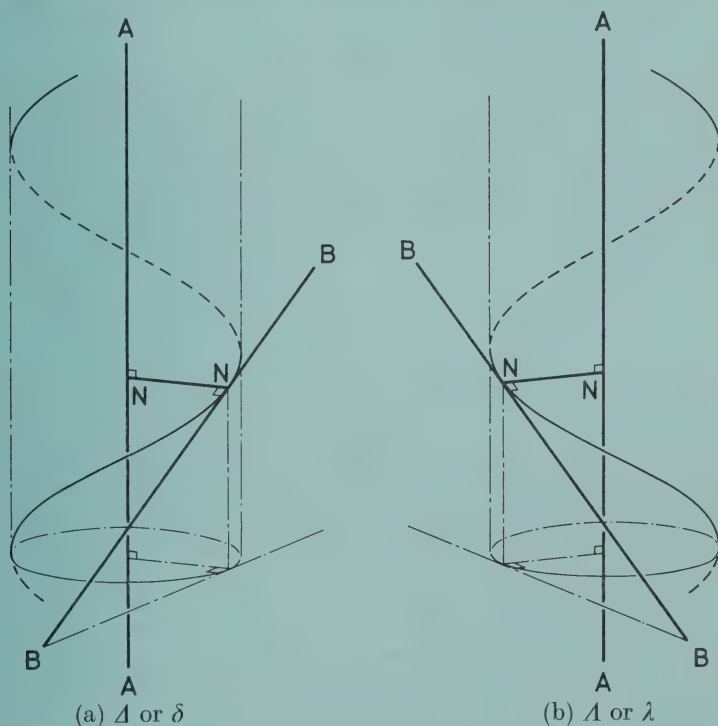


Fig. 2 Two skew lines *AA* and *BB* which are not orthogonal define a helical system. In the figure *AA* is taken as the axis of a cylinder whose radius is determined by the common normal *NN* of the two skew lines. The line *BB* is a tangent to the above cylinder at its crossing point with *NN* and defines a helix upon this cylinder by being the tangent to it at this crossing point. (a) and (b) illustrate a right- and a left-handed helix

lines AA determines the axis of a helix upon a cylinder whose radius is equal to the length of the two skew lines' common normal NN . The other of the skew lines BB makes up a tangent to the helix at N and determines the steepness of the helix. In Fig. 3 the two skew lines AA and BB are seen in projection on to a plane orthogonal to their common normal.

(a) of Fig. 2 and 3 illustrates a right-handed helix to be associated with the Greek letter delta (Δ referring to configuration, δ to conformation). (b) of Fig. 2 and 3 illustrates a left-handed helix to be associated with the Greek letter lambda (Λ for configuration, λ for conformation)*.

Because we are only interested in a qualitative measure of the helicity, the steepness of a helix is, in general, of no importance. However, the singularities at infinite steepness, where the skew lines become parallel lines, and at vanishing steepness, where the lines become orthogonal, should be noted. Here an infinitely small rotation of one line relative to the other about their common normal will change the helicity from right-handedness to left-handedness or vice versa. It is obvious that as the representation of our physical situation approaches these singularities the helicity becomes undefined (see Fig. 13).

3. Application to configuration

3.1 Representation to chelate rings

A chelate ring of a six-coordinated complex, whose ligators form an approximate octahedron, is represented by the edge determined by its two ligators. If two such edges are skew the pair can, without any further conventions, be associated** with either (a) or (b) of Fig. 3. This is the basis of the present proposal for nomenclature of absolute configurations.

Cis-bis-bidentate and tris-bidentate systems.

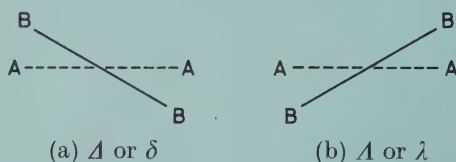


Fig. 3 The figure shows pairs of non-orthogonal skew lines in projection upon a plane parallel to both lines. The fully drawn line BB is above the plane of the paper, the dotted line AA below this plane. (a) corresponds to (a) of Fig. 2 and defines a right-handed helix. (b) corresponds to (b) of Fig. 2 and defines a left-handed helix

* It should be noted that orthogonal to the common normal of the two skew lines there is a two-fold axis (in fact, there are two such axes) of proper rotation which brings each one of the skew lines into coincidence with the other. This means that the helix which the first line, BB , say, determines around the second one, AA , has the same helicity as that which the second one determines around the first one.

** In connection with the singularities mentioned above it should be noted that by moving the ligators away from the ideal octahedral positions a gradual transition from the situation of Fig. 3 (a) to that of Fig. 3 (b) is possible without a change of absolute configuration. However, for this to occur the distortions must be so great that one would no longer think of calling the complex octahedral. Further such cases are unknown.

Two heavy line edges which are neither neighbouring edges having a common vertex, nor opposite edges, will in an octahedron form a pair of skew lines. This pair always has the same relative position as that of a *cis*-bis-bidentate complex.

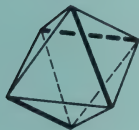
In Fig. 4 is seen the representation of the *cis*-bis-bidentate complex of Fig. 1 (b) redrawn so as to conform to Fig. 3, and for the particular absolute configuration to Fig. 3 (a). To the corresponding tris complex [Fig. 1 (a)] is attributed the same designation because its three heavy line edges are equivalent and therefore also the three possible pairs of heavy line edges. This is illustrated in Fig. 5.



Fig. 4 The bis-bidentate complex of Fig. 1 (b) redrawn so as to become associated with Fig. 3 (a) and thus to become designated by Δ



(a) Δ



(b) Δ



(c) Δ



(d) Δ



(e) Δ

Fig. 5 (a) and (b) show the tris-bidentate system of Fig. 1 (a) redrawn in two different ways. Since each of the bidentate ligands has lost its individuality by being represented only by the edge which it spans, the threefold axis of symmetry of the octahedron applies also to the present system. (a) shows the system in projection on a plane orthogonal to its threefold axis.

(c), (d), and (e) each illustrates one of the three possible pairs of bidentate ligands oriented so as to refer to (b). (c) is associated with Fig. 3 (a), and thus is designated by Δ . The same must hold true also for (d) and (e) because the threefold axis makes the three pairs of representations of bidentate ligands equivalent

3.2 Some examples of polydentate systems

It is straightforward to extend the application of the above rules to more complex situations involving polydentate ligands. It is by analogy with the tris-bidentate case (Fig. 5) only a matter of studying the interrelations between all the chelate rings whose corresponding edges form a pair of skew lines, *i.e.* all the ring pairs whose relative position is the same as in a *cis*-bis-bidentate complex. Now one might count up all such contributions and designate the complex situation by Δ if the number of Δ contributions from

the individual pairs exceeds the number of Δ contributions and vice versa. This convention, which could be applied to the situations shown in Fig. 6–8, will *not* be recommended here for the reason given in the next paragraph. Even though non-helical situations will always contribute Δ and Δ an equal number of times (Fig. 9), the same may be true as well for certain helical situations, as illustrated in Fig. 10.

A case such as that of Fig. 10 requires a further convention and here no simple one has yet been proposed. A possible convention here might conflict with the above simple counting of Δ and Δ contributions. We therefore recommend, at the present stage, for the case of Fig. 6–8 where the number of Δ and Δ contributions is different, to characterize the complexes as follows: Fig. 6, “skew chelate pair, Δ ”; Fig. 7, “skew chelate pair, Δ ”; Fig. 8, “skew chelate pairs, $\Delta\Delta\Delta$ ”. In the last example the order of the Greek letter symbols is immaterial. The case of Fig. 10 might at present be characterized by (“the end chelate rings form a skew chelate pair, Δ ”).

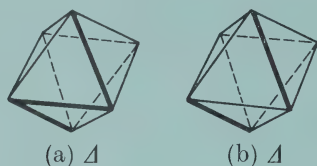


Fig. 6 A quadridentate system (a). Here only two of the heavy line edges are skew, the pair (b) being associated with Fig. 5 (d) and thus being designated by Δ . The system as a whole is proposed designated “skew chelate pair, Δ ”. The system may be thought of as representing the α -isomer of a trien-complex (trien = triethylenetetramine)

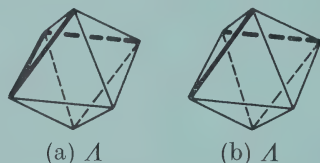


Fig. 7 Another quadridentate complex (a). As in Fig. 6 there is only one helical pair (b). This is clearly associated with the mirror image of Fig. 5 (c) (and, of course, therefore, also of Fig. 5 (d) and (e), although this is less easy to see) and thereby gives rise to the designation Δ . The system is therefore designated “skew chelate pair, Δ ”. The system may represent the β -isomer of a trien-complex (see Fig. 6)

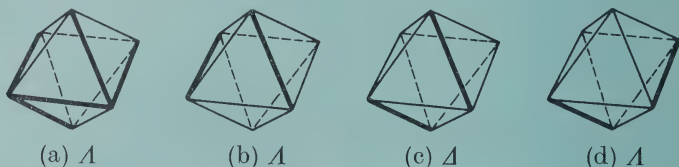


Fig. 8 A sexidentate complex (a). The pair (c) is associated with Fig. 5 (d) and is therefore Δ . The pairs (b) and (d) are clearly the mirror images of Fig. 5 (c) and 5 (e), respectively, and are therefore both Δ . The whole system is designated “skew chelate pairs, $\Delta\Delta\Delta$ ” where the order of the symbols is immaterial. The system may represent an EDTA complex (EDTA = Ethylenediaminetetraacetic acid)



Fig. 9 A non-helical system (a). The helical pairs (b) and (c) are mirror images of each other and contribute Δ and Λ , respectively. Non-helical systems always have an equal number of Δ and Λ contributions. The reverse conclusion, however, is not valid (see Fig. 10)



Fig. 10 A quinquidentate system (a). (b) is Δ by association with Fig. 5(c), (c) is Λ because it is the mirror image of (b).

A designation for the whole helical system (a) cannot be obtained without a further convention. A preliminary designation might be "the end chelate rings form a skew chelate pair, Λ "

4. Application to conformation

In order to define the helicity of a ring conformation a convention is required for making a choice of a pair of skew lines. Here it is proposed to choose one of the lines of this pair as the edge covered by the chelate ring, i.e. the line AA joining the two ligators. The other line BB is taken as that joining the two ring atoms which are neighbours to each of the ligators.

Two enantiomeric situations are shown in projection in Fig. 11. The two ligators AA are in the plane of the paper, the central atom M is below this plane and the two neighbouring ring atoms BB are above it. Fig. 11 (a) and (b) are associated with the corresponding Fig. 3, and the proposed convention for designating the helicity is thereby given. In Fig. 12 is shown a situation to which is attributed the same designation as that of the case of Fig. 11 (a). In Fig. 13 BB is parallel to AA and the chelate ring will not be helical at least up to a ring size of seven or eight members, which for our purpose is without importance. The situation in which BB is parallel to AA corresponds to the case of any planar chelate ring, and in addition to this, for a five-membered ring, it corresponds to the envelope form, and for the six-membered ring, either to the chair or to the boat form. In this case only the skew-boat form has a helical character.

Non-helical situations may still represent chiral situations when the chemical significance of the atoms, i.e. their possibility of being different, is considered. The present nomenclature problem, however, is not concerned with such cases.

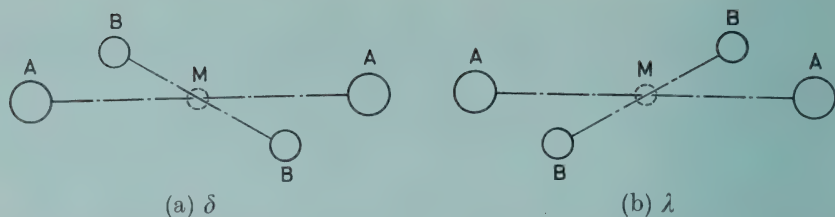


Fig. 11 Illustration of the convention for designating the helical character of the conformation of chelate rings. The ligating atoms in the plane of the paper determine one of our skew lines AA . The neighbouring-atoms of each ligator determine the other line BB , which here is above the plane of the paper, the central atom M being below this plane. The designations become clear by comparison with Fig.3 (a) and (b)

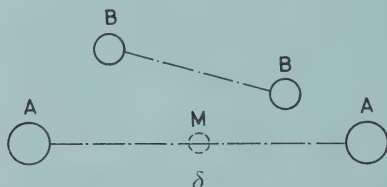


Fig. 12 Illustration of an alternative situation to that of Fig.11 (a). Both atoms BB are above the plane determined by M and AA , but this is immaterial from a nomenclature point of view. The lines AA and BB are still skew and correspond to the situation of Fig.3 (a)

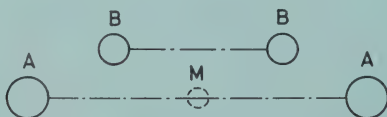


Fig. 13 Non-helical chelate ring drawn as in Fig.11. This figure illustrates a five-membered ring in its envelope form or a six-membered ring in either its boat or its chair form

5. Examples of a few absolute configurations

The proposals which have been put forward here dictate that the absolute configuration of the tris(ethylenediamine)cobalt(III) ion with a positive rotation at the Na_D line be characterized as upper case Λ and (—)propylenediamine in its stable chelate conformer (equatorial CH_3 -) be characterized by lower case λ .

6. Phenomenological characterization

As well as the symbols for designating structure some phenomenological description of a mirror-image isomer is essential. The isomer might be denoted by its sign of rotation at a particular wavelength, $(+)_\lambda$,

e.g., $(+)_\lambda [\text{Co}(\text{en})_3]\text{Cl}_3$ en = ethylenediamine

When optically active ligands are coordinated they are denoted as (+) and (−) where the signs are the signs of rotation of the ligand at the Na_D line,

e.g., (−)₅₈₉[Co{(−)pn}₃]Cl₃ pn = propylenediamine

In those instances where the absolute configuration of the ligand is known this might also be included in the description,

e.g., (−)₅₈₉[Co{(R)(−)pn}₃]Cl₃

7. Full characterization

Examples of the use of the full nomenclature proposed here follow:

Δ (+)₅₈₉[Co{(+)pn}₂{(−)pn}δδλ]Cl₃

(−)₅₈₉(Δ)(−)₅₈₉[Co{(R)(−)pn}₃λλλ](+)₅₄₆[Rh{C₂O₄}₃]
pn = propylenediamine

8. Rules for the designation of configurational chirality caused by chelation in six-coordinated complexes based on the octahedron

8.1 *Cis-bis-bidentate chelation*

The two ligating atoms of a chelate ring define a line. Two such lines for the pair of chelate rings define a helix. One line is the axis of the helix and the other is the tangent of the helix at the common normal for the skew lines. The tangent describes a right-handed (Δ) or a left-handed (Λ) helix with respect to the axis and thereby defines the configuration.

8.2 *Tris-bidentate chelation*

Any one of the three possible pairs of chelate rings is chosen to designate the configuration by rule 1.

8.3 *Multidentate chelation*

Chiral complexes of multidentate ligands are considered to contain pairs of skew lines (rule 1) and are designated by all the symbols, Δ 's and Λ 's, belonging to all the skew-line pairs. The order of citation of the symbols is immaterial.

9. Rule for the designation of conformational chirality of a chelate ring

The line joining the two ligating atoms and the line joining the two atoms of the chelate ring adjacent to each of the ligating atoms define a helix. One line is the axis of the helix and the other is the tangent of the helix at the common normal for the skew lines. The tangent describes a right-handed (δ) or a left-handed (λ) helix with respect to the axis and thereby defines the conformation.

Appendix

Relationship between the proposed symbols and those in earlier use

The symbols Δ and Λ were originally proposed for tris-bidentate complexes by PIPER¹ who used the threefold axis (C_3) as reference axis. The present convention agrees with the results of PIPER's proposal. The present convention for designation of conformation likewise agrees with LIEHR's² proposed use of δ and λ .

The absolute configuration³ of $(+)_589[\text{Co}(\text{en})_3]^{3+}$ (in the crystal, $\Delta \delta\delta\delta$) is Δ and that⁴ of $(-)_589[\text{Co}\{(-)\text{pn}\}_3]^{3+}$ is $\Delta \lambda\lambda\lambda$, as determined by SAITO *et al.* from X-ray crystallography. These two complex ions were in the X-ray papers designated by D and L , respectively. MASON pointed out that the helical configuration about a C_2 axis of a tris-bidentate or *cis*-diacidobis-bidentate complex is opposite to that about the respective C_3 or pseudo C_3 axes. He proposed⁵ the use of P (positive for right-handed) and M (minus for left-handed) as in $P(C_3)$ or $M(C_2)$ where the reference axis is indicated. The result of the present proposal is equivalent to that using the C_3 or pseudo C_3 axis and is *opposite* to that using a C_2 axis, i.e., Δ for $P(C_3)$ or $M(C_2)$ and Λ for $M(C_3)$ or $P(C_2)$. HAWKINS and LARSEN⁶ defined an octant sign to characterize the helicity of configurations (also of polydentate systems) as well as for conformations. For tris-bidentate and *cis*-bis-bidentate systems and for conformations of five and six-membered rings the relation to the present proposal is Δ (positive octant sign), λ (negative octant sign). LEGG and DOUGLAS⁷ suggested the general use of the C_2 axis for reference of helicity and a ring-pairing method for assigning the helicity of complexes containing polydentate ligands. The ring pairs chosen to define the helicity are the same as those proposed here. However, because of the C_2 -reference axis their use of Δ and Λ is opposite to that of the present proposal. It should further be noted that both the octant-sign method and the ring-pairing method of characterizing absolute configurations need extra conventions in certain cases of the type discussed here along with Fig. 10.

COREY and BAILAR⁸ and SARGESON⁹ have discussed the concomitant interplay of conformation and configuration in tris-bidentate diamine complexes. These authors designated the conformation of the five-membered ethylenediamine ring as k and k' , but used k and k' in the opposite sense*. With reference to our Fig. 11 the interrelation of δ , λ and k , k' is

COREY and BAILAR		SARGESON
δ	k'	k
λ	k	k'

Acknowledgment: The Commission wishes to express its appreciation of the valuable help offered by Dr. WERNER FENCHEL, professor of mathematics at the University of Copenhagen, by Sir CHRISTOPHER INGOLD and Dr. R. S. CAHN, and by several chemists working with optically active complexes.

* The cause of the confusion with respect to k and k' is an error in the upper drawing of Fig. 3 of COREY and BAILAR's paper!. The ring conformations of the unstable form, the *ob* form $\Delta \delta\delta\delta$, is correctly given as $k'k'k'$ in the lower drawing of their Fig. 3, but the stable form, the *lel* form $\Delta \lambda\lambda\lambda$, discussed in the text correctly as kkk , appears in the upper drawing of their Fig. 3 as $\Delta \delta\delta\delta$

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- 5 McCaffery, A.J./Mason, S.F./Ballard, R.E.: *J.Chem.Soc.* 1965, 2883;
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- 8 Corey, E.J./Bailar, J.C., jr.: *ibid.*, 81, 2620 (1959)
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ker, New York, 3, 303 (1966)

CALENDAR

* = not sponsored by IUPAC

Under the pressure of time, it was not possible to establish a detailed new calendar because not all questions of IUPAC sponsorship were settled at the time of printing this Information Bulletin. The Calendar as printed in Information Bulletin No. 32 is reprinted with a proviso.

1969

February 2-9	X Congreso latinoamericano de Química	San José (Costa Rica)
April 21-25	Symposium on Natural Products, in particular Steroids and Terpenes	México City (México)
May 27-30	Société de Chimie Physique	Paris (France)
July 4-8	XXVth International Conference of Pure and Applied Chemistry	Cortina d'Ampezzo (Italy)
July 14-18	IVth International Congress of Pharmacology	Basle * (Switzerland)
July 14-18	International Conference on Atomic Absorption Spectroscopy	Sheffield (UK)
July 14-20	International Symposium on Chemical Control of Human Environment	Johannesburg (S. Africa)
July 17-19	Symposium on Surface Area Determination	Bristol (UK)
July 21-25	International Symposium on Analytical Chemistry	Birmingham (UK)
July 27-August 1	IVth International Symposium on Organometallic Chemistry	Bristol (UK)
August 20-27	XXIIInd International Congress of Pure and Applied Chemistry and XIIth International Conference on Coordination Chemistry	Sydney (Australia)
August 25-30	Symposium on Kinetics and Mechanism of Poly-reaction	Budapest (Hungary)
September 8-13	VIIIth International Congress of Clinical Chemistry	Geneva (Switzerland)
September 9-12	International Symposium on Conformational Analysis	Brussels (Belgium)
To be decided	Symposium on Nonaqueous Electrochemistry	To be decided *
1969 or 1970	Cyclo-Addition	Munich (Germany)

1970

Beginning	Analytical Congress	Budapest (Hungary)
July	VIth International Symposium on Chemistry of Natural Products	Riga (USSR)
	VIth International Symposium on Microchemistry	Graz (Austria)
	Symposium on Carbohydrate Chemistry (Division of Organic Chemistry)	
	Symposium on Macromolecular Physics (Macromolecular Division)	Leiden or Delft (Netherlands)
September 20-24	Conference on Analytical Chemistry	Budapest (Hungary)

1971

July	XXVIth International Conference of Pure and Applied Chemistry	Washington, DC (USA)
	XXIIIrd International Congress of Pure and Applied Chemistry	Boston (USA)
	Symposium on Macromolecular Chemistry	Boston (USA)

LIST OF ABBREVIATIONS

AOAC	Association of Official Agricultural Chemists
CBN	Commission on Biochemical Nomenclature
CEBJ	Commission of Editors of Biochemical Journals
CEE	Communauté Economique Européenne
CIG	Comité International de Géophysique
CIPM	Comité International de Poids et Mesures
CITCE	Comité International de Thermodynamique et Cinétique Electrochimique
CNRS	Centre national de la Recherche scientifique
COMECON	Council for Mutual Economic Assistance
COSPAR	Committee on Space Research
CSF	Compagnie Télégraphie Sans Fil
CSIRO	Commonwealth Scientific and Industrial Research Organization
DECHEMA	Deutsche Gesellschaft für chemisches Apparatewesen eV
EEC	European Economic Community
EMPA	Eidgenössische Materialprüfungs-Anstalt
EPPO	European and Mediterranean Plant Protection Organization
ETH	Eidgenössische Technische Hochschule (Zürich)
EUCEPA	European Committee on Cellulose and Paper
EUROTOX	Comité européen permanent pour la Protection des populations contre les risques de toxicité à long terme
FAGS	Fédération of Astronomical and Geophysical Services
FAO	Food and Agriculture Organization
GEFAP	Groupement européen des Associations nationales de Fabricants de Pesticides
IAEA	International Atomic Energy Agency
IAMS	International Association of Microbiological Societies
IAPT	International Association for Plant Taxonomy
IASH	International Association of Scientific Hydrology
IAU	International Astronomical Union
IBP	International Biological Programme
ICCA	International Commission for Cellulose Analysis
ICSU	International Council of Scientific Unions
ICUMSA	International Committee for the Unification of Methods of Sugar Analysis
IGU	International Geographical Union
IMU	International Mathematical Union
ISO	International Organization for Standardization

ITU	International Telecommunication Union
IUB	International Union of Biochemistry
IUBS	International Union of Biological Sciences
IUCr	International Union of Crystallography
IUGG	International Union of Geodesy and Geophysics
IUGS	International Union of Geological Sciences
IUNS	International Union of Nutritional Sciences
IUPAC	International Union of Pure and Applied Chemistry
IUPAP	International Union of Pure and Applied Physics
JCAM	Joint Commission on Atomic Masses
JCAR	Joint Commission on Applied Radioactivity
MIT	Massachusetts Institute of Technology
NAS	National Academy of Sciences
NATO	North Atlantic Treaty Organization
NBS	National Bureau of Standards
NRC	National Research Council
OECD	Organisation de Coopération et de Développement économiques
OEPP	Organisation européenne de Protection des Plantes
OMS	Organisation Mondiale de la Santé
SCAR	Scientific Committee on Antarctic Research
SCOR	Scientific Committee on Oceanic Research
UICC	Union internationale contre le Cancer
UNESCO	United Nations Educational Scientific and Cultural Organization
WHO	World Health Organization
WMO	World Meteorological Organization

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**INTERNATIONAL UNION OF PURE
AND APPLIED CHEMISTRY**

**UNION INTERNATIONALE DE CHIMIE
PURE ET APPLIQUÉE**

50 YEARS IUPAC

1918–1968

Corrected Tentative Rules


**INFORMATION BULLETIN
NUMBER 33**

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SECRETARY GENERAL:

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Cable address: IUPACAIRPORT

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It is greatly regretted that the Tentative Revised Rules for Steroid Nomenclature were printed in Information Bulletin No. 33 without the proofs having been corrected. They are therefore reprinted in this issue after correction by representatives of the two Commissions concerned.

BBA Rules 12

IUPAC Commission on the Nomenclature of Organic Chemistry and IUPAC-IUB Commission on Biochemical Nomenclature

REVISED TENTATIVE RULES FOR NOMENCLATURE OF STEROIDS*

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* These Rules shall be known as the IUPAC-IUB 1967 Revised Tentative Rules for Steroid Nomenclature.

These Rules are issued by the IUPAC Commission on the Nomenclature of Organic Chemistry (P. E. VERKADE (Chairman), L. C. CROSS, G. M. DYSON, K. L. LOENING, N. LOZAC'H, H. S. NUTTING, J. RIGAUDY, S. VEIBEL; Associate members: R. S. CAHN, S. P. KLESNEY; Observers: K. A. JENSEN, W. KLYNE), and by the IUPAC-IUB Commission of Biochemical Nomenclature (O. HOFFMANN-OSTENHOF (Chairman), A. E. BRAUNSTEIN, W. E. COHN, J. S. FRUTON, P. KARLSON, B. KEIL, W. KLYNE, C. LIÉBECQ, E. C. SLATER, E. C. WEBB; Corresponding member: N. TAMIA; Observer: S. VEIBEL).

Comments on and suggestions for future revisions of these Tentative Rules should be sent to: Professor P. E. VERKADE, Ary Schefferstraat, 217, 's-Gravenhage, The Netherlands, or Professor O. HOFFMANN-OSTENHOF, Biochemische Abteilung, Organisch-Chemisches Institut der Universität Wien, Währingerstrasse 38, 1090 Vienna, Austria, or to any member of the Commissions named above. Reprints of these Revised Tentative Rules may be obtained from the NAS-NRC Office of Biochemical Nomenclature (Dr. WALDO E. COHN, Director), Biology Division, Oak Ridge National Laboratory, Oak Ridge, Tenn. 37830, U.S.A.

IUPAC Commission on the Nomenclature of Organic Chemistry and IUPAC-IUB Commission on Biochemical Nomenclature

REVISED TENTATIVE RULES FOR NOMENCLATURE OF STEROIDS

INTRODUCTION

The rules of steroid nomenclature originate from a discussion held at the Ciba Foundation in London, England, in 1950 between the representatives of many schools. These were published in *Chem. Ind. London*, (1951) p. SN 1-11, and also in French and German. They were subsequently taken over by the International Union of Pure and Applied Chemistry and published in an official form in the *Comptes Rendus* of the Zurich meeting in 1952 (also *IUPAC Nomenclature of Organic Chemistry, Sections A and B*, 1957, Butterworths, London, 1st ed. 1958; 2nd ed. 1966, p. 71-82; and numerous reprints and translations, including *J. Am. Chem. Soc.*, 82 (1960) 5577).

In 1960 a group of specialists under the chairmanship of Professor T. REICHSTEIN, including representatives of the IUPAC Commissions on the Nomenclature of Organic Chemistry and of Biochemical Nomenclature, met in Basle, Switzerland, for discussions of amendments and additions to the Rules. Agreement was not reached on all the points discussed, and the results of this meeting were therefore published in discussion form in the *IUPAC Information Bulletin*, No. 11. They have generally been referred to as the "Basle Proposals".

Since then, many points in the Basle Proposals have become almost universally accepted in the literature. In 1965 the two International Commissions concerned, namely, the IUPAC Commission on the Nomenclature of Organic Chemistry and the Commission on Biochemical Nomenclature (now jointly responsible to IUPAC and IUB), decided that the time had come for as many as possible of the Basle Proposals to be formulated as rules.

The present Rules include: all the original Rules, mostly renumbered (with additions and amendments arising from the Basle Proposals or from current practice in the literature); and most of the Basle Proposals, namely, those that have been generally accepted. Further, adoption of the sequence-rule procedure* for general

* R. S. CAHN, C. K. INGOLD AND V. PRELOG, *Angew. Chem. Intern. Ed.*, 5 (1966) 385 (in English); *Angew. Chem.*, 78 (1966) 413 (in German); for a partial simplified account see R. S. CAHN, *J. Chem. Educ.*, 41 (1964) 116.

stereochemical descriptions in much of the chemical literature has permitted its introduction now also for some sections of steroid nomenclature that were previously in dispute or intractable. Decisions on a few of the Basle Proposals have, however, been postponed; it is hoped that further experience will indicate the most appropriate ways of dealing with them.

General application

Although these Rules are called "Rules for Nomenclature of Steroids", many of the principles therein have become almost universally accepted also in diterpene and triterpene chemistry; also to some extent for sesquiterpenes and for several groups of alkaloids. It is suggested that the same principles may be applied to a number of other specialized groups of natural products, perhaps without the need for further official rules, so long as the basic ideas are followed. These principles include: (i) clear definition of stem names and the stereochemistry implied in them; (ii) systematic application of the rules of general organic chemical nomenclature, with modifications where special considerations make this necessary; (iii) application of the methods of skeletal modification given in these Rules, *viz.*, the use of homo and nor for, respectively, stepwise expansion and contraction of ring systems; the use of seco for reductive fission of ring systems; and the use of *abeo* for formal bond migrations (this flexible concept was first proposed by Professor D. H. R. BARTON at an informal meeting of terpene chemists convened by the Chemical Society in London, England).

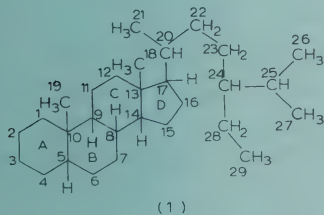
RULES

Rules are numbered 2S-1, 2S-2, 2S-3, *etc.*, the first "2" denoting that this is the second or revised set of rules. The numbers of the corresponding previous rules, where they exist, are included for comparisons.

General

Rule 2S-1 (expanded from Rules S-1 and S-2)

1.1. Steroids are numbered and rings are lettered as in Formula (1). If one of the two methyl groups attached to C-25 is substituted it is assigned the lower



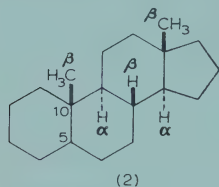
number (26); if both are substituted, that carrying the substituent cited first in the alphabetical order or order of complexity is assigned the lower number (*cf.* IUPAC Rule* C-15.11(e)). For trimethyl steroids see Rule 2S-2.3, Note b.

* IUPAC Nomenclature of Organic Chemistry, Section C, 1965, Butterworths, London; also *Pure Appl. Chem.*, 11, No. 1 and 2 (1965).

1.2. If one or more of the carbon atoms shown in (1) is not present and a steroid name is used, the numbering of the remainder is undisturbed.

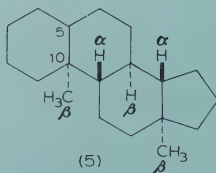
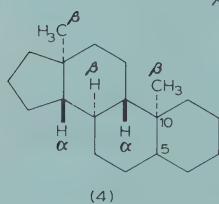
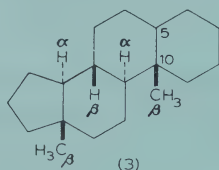
1.3. For a steroid the name, including stereochemical affixes, and its structural formula (see Rule 2S-1.4), denote the absolute configuration at each asymmetric centre (see also Rule 2S-1.5). When the configuration at one or more centres is not known, this is indicated by Greek letter(s) ξ (xi) prefixed by the appropriate numeral(s).

1.4. When the rings of a steroid are denoted as projections onto the plane of the paper, the formula is normally to be oriented as in (2). An atom or group attached to a ring depicted as in the orientation (2) is termed α (alpha) if it lies below the plane of the paper or β (beta) if it lies above the plane of the paper. In formulae,



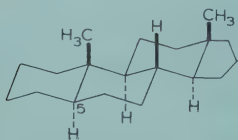
bonds to atoms or groups lying below the plane of the paper are shown as broken (---) lines, and bonds to atoms or groups lying above the plane of the paper are shown as solid lines (preferably thickened —). Bonds to atoms or groups whose configuration is not known or is unspecified are denoted by wavy lines (~~~~).

Notes: (1) Projections of steroid formulae should not be oriented as in Formula (3), (4), or (5) unless circumstances make it obligatory.

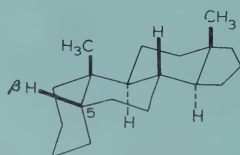


(2) With the preferred orientation (2), and with (3), α bonds appear as broken lines and β bonds as solid (thickened) lines. The reverse is true for (4) and (5). Wavy lines denote ξ bonds for all orientations of the formula.

(3) A perspective representation of the stereochemistry of Formula (2) as in (2a) or (2b) may also be used.



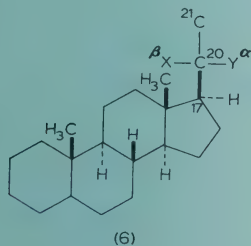
A 5 α -steroid



A 5 β -steroid

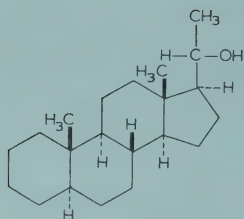
(For the significance of the prefixes 5 α - and 5 β - see Rule 2S-1.5.)

1.6. When the configuration at position 20 in the side chain of a pregnane derivative* is as depicted in the projection formula (6) (*i.e.*, a Fischer projection but with the highest number at the top), substituents shown to the right of C-20 are termed α and those to the left are termed β .



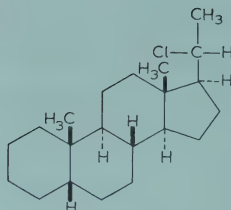
Biochim. Biophys. Acta, 164 (1968) 453-486

Examples:



(7)

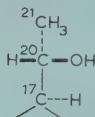
5α-Pregnan-20α-ol*



(8)

20β-Chloro-5β-pregnane*

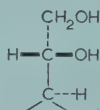
Notes: (1) The 20α/20β-nomenclature is continued because of long tradition. When a longer side chain is present at C-17 the sequence-rule procedure (for references, see footnote on p. 454) is more generally convenient (see Rule 2S-1.7) and it may also be used to designate stereochemistry at C-20 in pregnanes, being particularly useful for 20-substituents that may cyclize with a substituent at another position (*e.g.*, carboxylic acids as in Example (12)). For 20-hydroxy-, 20-alkoxy-, 20-acyloxy-, 20-amino-, and 20-halogeno- derivatives of pregnane without a substituent on C-17 or C-21, 20α- is equivalent to (20*S*)-, and 20β- to (20*R*)-; however, these equivalences are sometimes reversed when additional substituents are present, *e.g.*, on C-17 or C-21, and in such cases the references in the footnote, p. 454 should be consulted.



(9)

20α-ol (20*S*)

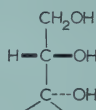
but



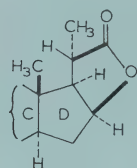
(10)

20α,21-diol (20*R*)

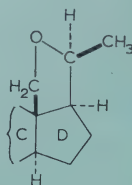
although



(11)

17,20α,21-triol (20*S*)

(12)

(20*S*)-16β-Hydroxypregnane-20-carboxylic acid lactone (≡ 20α)

(13)

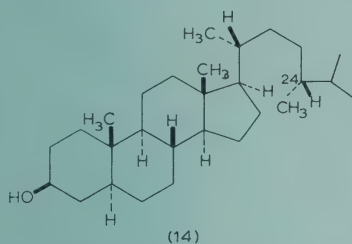
(20*S*)-18,20-Epoxypregnane (≡ 20α)

(2) When stereochemistry at C-20 is denoted by a Fischer-type projection, as in (6)–(11) or for cardenolides as (37) or bufanolides as (43), the 17,20-bond is preferably denoted by an ordinary line; the stereochemistry at C-17 is then adequately denoted by a thick or a broken bond to the H or to the other substituent (*e.g.*, OH) at position 17. In such formulae, representing the 17,20-bond by a thick or a broken line cannot be correct for both C-17 and C-20; this has, however, frequently been done, then involving the additional convention that the way in which this bond is written is neglected when considering the stereochemistry at C-20.

* For the name "pregnane" see Rule 2S-2.3.

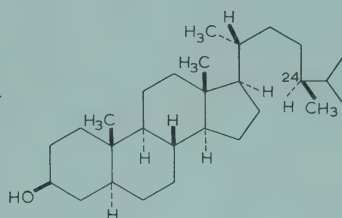
1.7. The stereochemistry at C-20 and other positions in steroid side chains longer than ethyl is described by the sequence-rule procedure (for references, see footnote on p. 454).

Examples:



(14)

(24*R*)-24-Methyl-5 α -cholestan-3 β -ol*
(formerly 24 α -methyl)
(trivial name: campestanol)



(15)

(24*S*)-24-Methyl-5 α -cholestan-3 β -ol*
(formerly 24 β -methyl)
(trivial name: ergostanol)

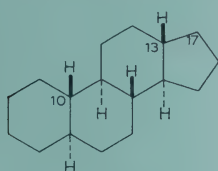
Notes: (1) The sequence-rule procedure is also used when the side chain is cyclized (see Rules 2S-3.3 and 2S-3.4).

(2) The backbone of a 17-side chain is best denoted as in the plane of the paper (lines of ordinary thickness), the 17,20-bond being similarly denoted. Except for pregnane derivatives, stereochemistry due to substituents on the chain is then indicated by the customary thick or broken lines denoting bonds that project, respectively, above and below the plane of the paper.

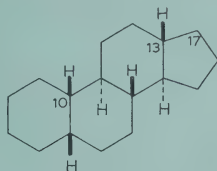
Fundamental carbocycles

Rule 2S-2 (expanded from Rules S-3.1 to S-3.5)

2.1. The parent tetracyclic hydrocarbon without methyl groups at C-10 and C-13 and without a side chain at C-17 is named "gonane".



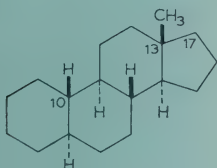
(16)

5 α -Gonane

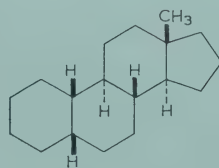
(17)

5 β -Gonane

2.2. The hydrocarbon with a methyl group at C-13 but without a methyl group at C-10 and without a side chain at C-17 is named "estrane".



(18)

5 α -Estrane

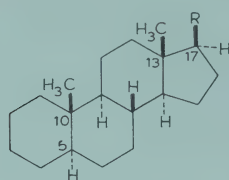
(19)

5 β -Estrane

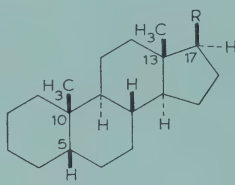
* For the name "cholestane" see, Rule 2S-2.3. These systematic names are preferred to the trivial names given below them.

Note: Names of compounds having a methyl group attached to C-10 and a hydrogen atom attached to C-13 are to be based on 18-norandrostane (see Rules 2S-2.3 and 2S-7.1) and not on 10-methylgonane.

2.3. The following names are used for the hydrocarbons (20) and (21) with methyl groups at both C-10 and C-13.



(20)



(21)

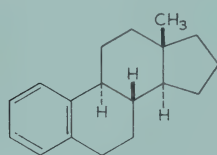
R	(20) 5 α -Series	(21) 5 β -Series
H	5 α -Androstane	5 β -Androstane (not testane)
C ₂ H ₅	5 α -Pregnane (not allopregnane)	5 β -Pregnane
* CH(CH ₃)CH ₂ CH ₂ CH ₃	5 α -Cholane (not allocholane)	5 β -Cholane
* CH(CH ₃)CH ₂ CH ₂ CH ₂ CH(CH ₃) ₂	5 α -Cholestane	5 β -Cholestane (not coprostate)
* CH(CH ₃)CH ₂ CH ₂ CH ^{24**} (CH ₃)CH(CH ₃) ₂	5 α -Ergostane	5 β -Ergostane
* CH(CH ₃)CH ₂ CH ₂ CH ^{24***} (C ₂ H ₅)CH(CH ₃) ₂	5 α -Stigmastane	5 β -Stigmastane

* 20R Configuration.

** 24S Configuration.

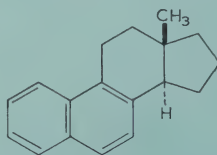
*** 24R Configuration.

Notes: (a) Unsaturation and substituents are denoted in the names of steroids by the usual methods of organic chemistry (*cf.* Rule 2S-4). Examples (22)–(25) illustrate some simple cases.



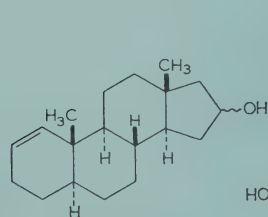
(22)

1,3,5(10)-Estratriene

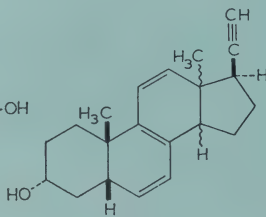


(23)

1,3,5(10),6,8-Estrapentaene



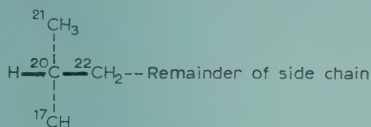
(24)

5 α -Androst-1-en-16 ξ -ol

(25)

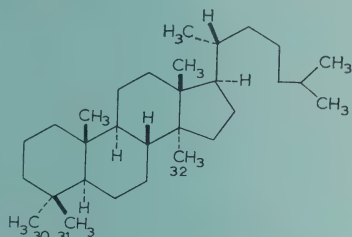
5 β ,13 ξ ,14 ξ -Estrapenta-6,8,11-trien-20-yn-3 α -ol

(b) The names "cholane", "cholestane", "ergostane", and "stigmastane" imply the configuration at C-20 shown in partial formula (26); this is (20*R*) except for some derivatives containing additional substituents (*cf.* Notes to Rule 2S-1.6).

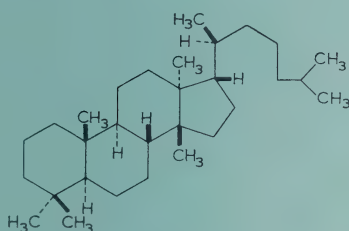


(26)

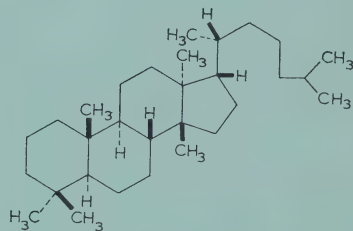
(c) Tetracyclic triterpenoids may be regarded as trimethyl steroids, the three additional methyl groups being numbered 30 (attached to C-4 with α configuration), 31 (attached to C-4 with β configuration), and 32 (attached to C-14); for example, 5 α -lanostane (27) is 4,4,14 α -trimethyl-5 α -cholestane, the former name implying 14 α , 20*R* configuration. Trivial names are common in this series of compounds, and some are illustrated in Examples (27)–(31).



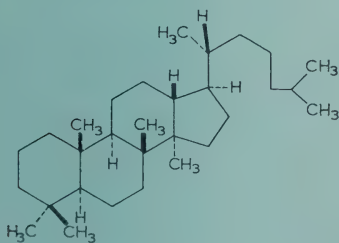
(27)

5 α -Lanostane

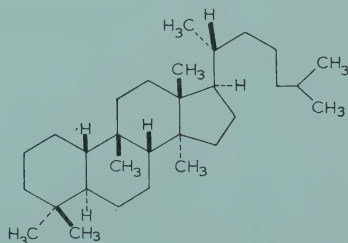
(28)

5 α -Tirucallane5 α , 13 α , 14 β , 17 α , 20*S*-Lanostane

(29)

5 α -Euphane5 α , 13 α , 14 β , 17 α -Lanostane
(20*R* implied in the name)

(30)

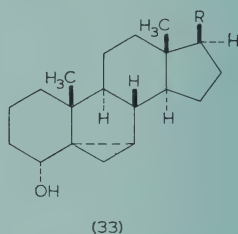
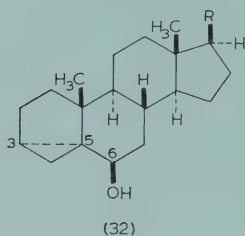
5 α -Dammarane8-Methyl-18-nor-5 α -lanostane (all configurations except 5 α are implied in the name)

(31)

5 α -Cucurbitane19(10 \rightarrow 9 β)-abeo-5 α -Lanostane (for the *abeo* nomenclature see Rule 2S-9)

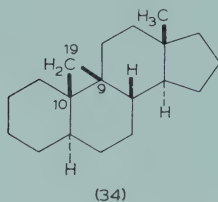
2.4. When an additional ring is formed by means of a direct link between any two carbon atoms of the steroid ring system or the attached side chain, the name of the steroid is prefixed by "cyclo"; this prefix is preceded by the numbers of the positions joined by the new bond and the Greek letter (α , β , or ξ) denoting the configuration of the new bond, unless that designation is already implicit in the name.

Examples:

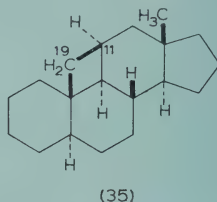


3 α ,5-Cyclo-5 α -cholestan-6 β -ol

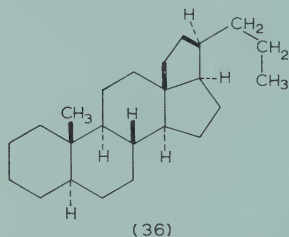
5,7 α -Cyclo-5 α -cholestan-4 α -ol



9,19-Cyclo-5 α ,9 β -androstane



11 β ,19-Cyclo-5 α -androstane



(20*R*)-18,21-Cyclo-5 α -cholane

Penta- and hexa-cyclic modifications

Rule 2*S*-3 (amended versions of Rules S-3.6 to S-3.9)

3.1. (a) The name "cardanolide" is used for the fully saturated system (37) of digitaloid lactones whose configuration is as illustrated (the configuration at position 20 is shown as a Fischer-type projection* and is the same as that in cholesterol, *i.e.*, 20*R*). Notwithstanding Rule 2*S*-1.5, the configuration at position 14 must always be stated as an affix to the names of these compounds.

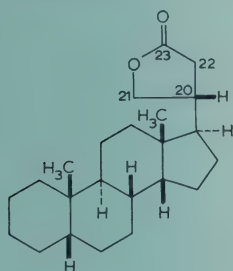
(b) Names such as "20(22)-cardanolide" are used for the naturally occurring unsaturated lactones of this type.

* This method of drawing is customary for the steroids. Since the highest-numbered atom is at the top, the usual Fischer projection has been rotated in the plane of the paper through 180°.

(c) The names "14,21-" and "16,21-epoxycardanolide" are used for the compounds containing a 14,21- or a 16,21-oxygen bridge, respectively.

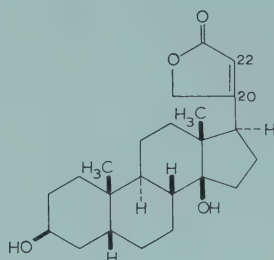
Note: Statement of the configuration at C-14 for all cardanolides is a change from the earlier steroid Rules and is in line with current practice.

Examples:

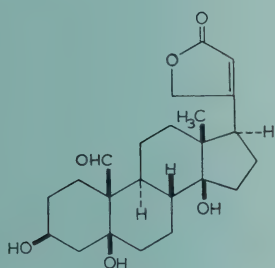


(37)

5β,14β-Cardanolide

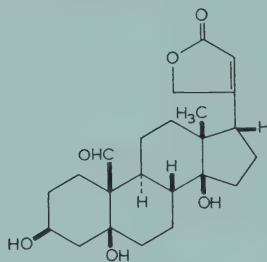


(38)

3β,14-Dihydroxy-5β,14β-card-20(22)-enolide
(= digitoxigenin*)

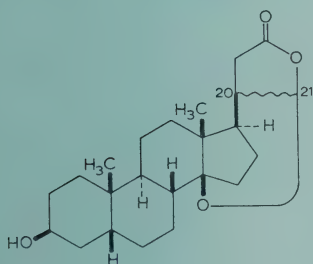
(39)

3β,5,14-Trihydroxy-19-oxo-5β,14β-card-20(22)-enolide (= strophanthidin*)



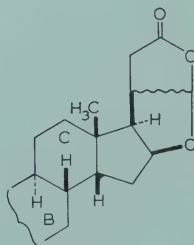
(40)

3β,5,14-Trihydroxy-19-oxo-5β,14β,17α-card-20(22)-enolide (= 17α-strophanthidin*) (also, allostrophanthidin**)



(41)

3β-Hydroxy-14,21ξ-epoxy-5β,14β,20ξ-cardanolide (= isodigitoxigenin**)



(42)

A 16β,21ξ-epoxy-14β,20ξ-cardanolide

3.2. The name "bufanolide" is used for the fully saturated system (43) of the squill-toad poison group of lactones, with the configuration at position 20 shown

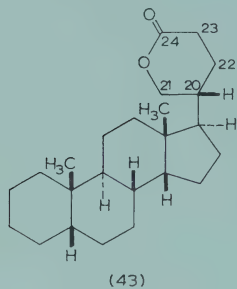
* Denotes a trivial name; the systematic name is preferred.

** Denotes a previous trivial name now considered unacceptable.

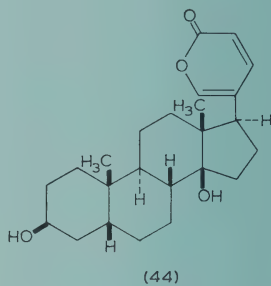
(this configuration is drawn as a Fischer-type projection (see Note to Rule 2S-3.1(a)) and is the same as in cholesterol, *i.e.*, 20*R*). Notwithstanding Rule 2S-1.5, the configuration at position 14 must always be stated as an affix to the names of these compounds. Unsaturated derivatives are named by replacing the suffix -anolide by -enolide, -adienolide, *etc.*; thus, the name "20,22-bufadienolide" is used for the naturally occurring doubly unsaturated lactones.

Note: Statement of the configuration at C-14 for all bufanolides is a change from the earlier steroid Rules and is in line with current practice.

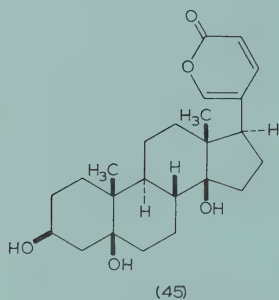
Examples:



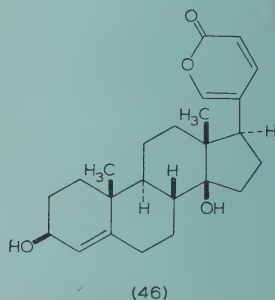
(43)
5 β ,14 β -Bufanolide



(44)
3 β ,14-Dihydroxy-5 β ,14 β -bufa-20,22-dienolide
(= bufalin*)



(45)
3 β ,5,14-Trihydroxy-5 β ,14 β -bufa-20,22-dienolide (= telecinobufagin*)



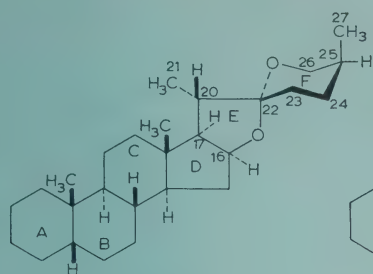
(46)
3 β ,14-Dihydroxy-14 β -bufa-4,20,22-trienolide
(= scillarenin*)

3.3. The name "spirostan" is used for the compound of structure (47) (this is a 16,22:22,26-diepoxycholestane); this name specifies the configurations shown for all the asymmetric centres except positions 5 and 25. A prefix 5 α - or 5 β - is added in the usual way (see Rule 2S-1.5). Configurations at C-16 and C-17, if different from those shown in Formula (47), are designated as 16 β (H) and 17 β (H). Configurations at C-20 and C-22, if different from those shown in Formula (47), are designated by the sequence-rule procedure** or, if unknown, by ξ . Steric relations of substituents at C-23, C-24, C-25, or C-26 are in all cases designated by the sequence-rule procedure** or, if unknown, by ξ .

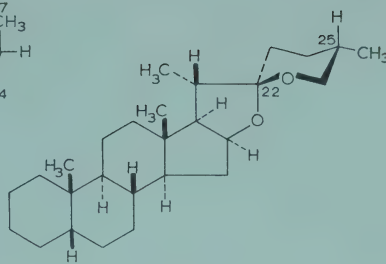
* Denotes a trivial name; the systematic name is preferred.

** For references, see footnote on p. 454.

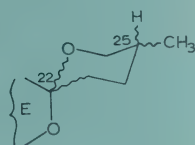
Examples:



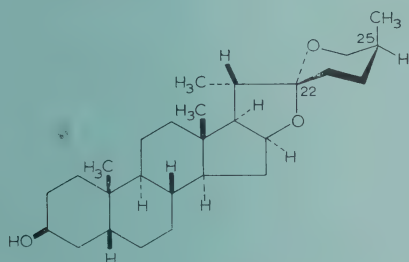
(47)
(25*S*)-5β-Spirostan



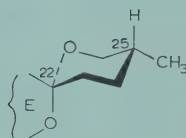
(48)
(22*S*,25*S*)-5β-Spirostan



(49)
22ξ,25ξ-



(50)
(25*S*)-5β-Spirostan-3β-ol
(= sarsapogenin*)



(51)
(25*R*)-

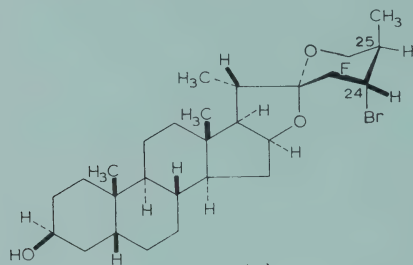
Notes: Several other methods have been used in the past for designating stereochemistry at C-22 and C-25 in the spirostans and related series; all involve serious difficulties (*cf. The Basle Proposals, IUPAC Inform. Bull.*, 11; also L. F. FIESER AND M. FIESER, *The Steroids*, Reinhold, New York, 1959, Chapter 21). The sequence-rule procedure is adopted in these Rules because it gives an unequivocal symbolism.

It is to be noted that, although ring E, like rings A, B, C, and D, can conveniently be shown by projection on to the plane of the paper, yet ring F cannot be adequately represented in this way since the oxygen atom, C-26, C-24, and C-23 lie in one plane that is perpendicular to the plane of the paper. Ring F is conveniently drawn as in Formulae (47)–(51); in Formula (47), for instance, the broken line from C-22 to oxygen denotes that the oxygen atom and C-26 of ring F lie behind the plane of the paper and that consequently C-23 and C-24 lie in front of the plane of the paper (configuration *R* at C-22). In partial formula (48) the configuration at C-22 is reversed and must be stated in the name (*S*). It is conventional to draw ring F as a chair, but this conformation is not implied in the name “spirostan”; whatever

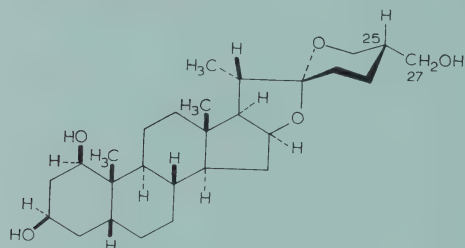
* Denotes a trivial name; the systematic name is preferred.

the conformation of ring F, C-27 and the 25-hydrogen atom both lie in the plane of the paper and so cannot be denoted by broken or thickened lines or designated α or β . In (47) the methyl group is axial (above the general plane of ring F), and in (48) it is equatorial (in the general plane of ring F); in both these cases the configuration at C-25 is *S*, but this identity of *R,S* designation arises only because the configuration at C-22 has also been reversed between (47) and (48); a 25*R* configuration is shown in (51). The wavy lines in (49) denote unspecified or unknown configurations at both C-22 and C-25.

The *R,S* specification may also be affected by substituents attached to ring F or C-27, as in Compounds (A) and (B).



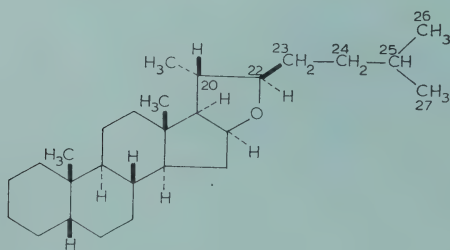
(A)
(24*R*)-Bromo-(25*R*)-5 β -spirostan-3 β -ol



(B)
(25*S*)-5 β -Spirostan-1 β ,3 β ,27-triol

3.4. The name "furostan" is used for the compound of structure (52) (16 β ,22-epoxycholestane); this name specifies the configurations at all the asymmetric centres except positions 5, 22, and (if position 26 is substituted) also 25. Configuration at C-5 is designated by use of α or β in the usual way (see Rule 2S-1.5), and configurations at C-22 and, if necessary, C-25 by the sequence-rule procedure, or in all these cases by ξ if unknown.

Example:

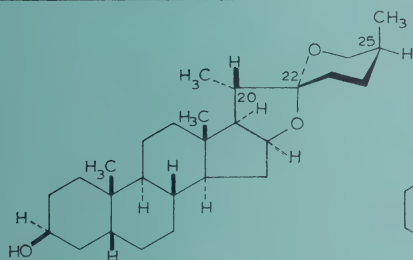


(52)
(22*R*)-5 β -Furostan

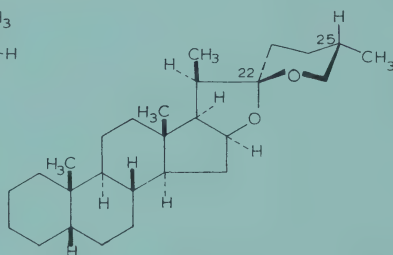
Note: Representative examples of the new standard names and old names (standard names are preferred) for some common types of spirostan, furostan, and derived structures are given in the following table and formulae.

SPIROSTANS AND FUROSTANS

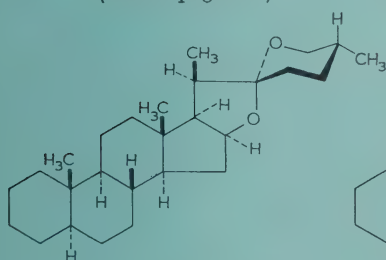
Formula type	Standard name	Configurations implied in standard name	Old names (with trivial names for particular compounds in brackets)*
47	(25 <i>S</i>)-Spirostan	20 <i>S</i> ,22 <i>R</i>	Sapogenin (without prefix) Neogenin 25- <i>L</i> -Genin [Sarsasapogenin is (53)]
51	(25 <i>R</i>)-Spirostan	20 <i>S</i> ,22 <i>R</i>	Isogenin 25- <i>D</i> -Genin [Smilagenin is (25 <i>R</i>)-5β-spirostan-3β-ol] Tigogenin is (25 <i>R</i>)-5α-spirostan-3β-ol]
54	(20 <i>R</i> ,22 <i>S</i> ,25 <i>S</i>)-Spirostan	—	Cyclopseudoneogenin (54)
55	(20 <i>R</i> ,22 <i>R</i> ,25 <i>R</i>)-Spirostan	—	Cyclopseudoisogenin (55)
56	(22 <i>R</i>)(or <i>S</i> or <i>ξ</i>), (25 <i>R</i>)(or <i>S</i> or <i>ξ</i>)-Furostan	20 <i>S</i>	Dihydrogenin (26-ol) and Dihydropseudogenin (26-ol) [Dihydrosarsasapogenin is 5β,22ξ,25 <i>S</i> -furostan-3β,26-diol Dihydropseudotigogenin is (58); cf. (57)]
57	(25 <i>R</i>)(or <i>S</i> or <i>ξ</i>)- Furost-20 (22)-en	—	Pseudogenin [Pseudotigogenin is (57) Pseudosarsasapogenin is (59) Pseudosmilagenin is (25 <i>R</i>)-5β-furost-20 (22)-en-3β,26-diol]



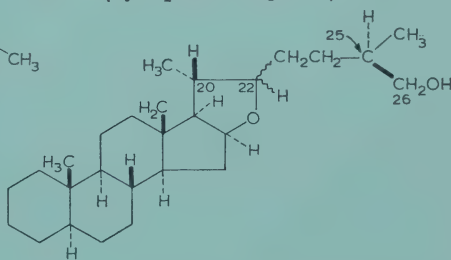
(53)
(25*S*)-5β-Spirostan-3β-ol
(Sarsasapogenin*)



(54)
(20*R*,22*S*,25*S*)-5β-Spirostan
(Cyclopseudoneogenin*)

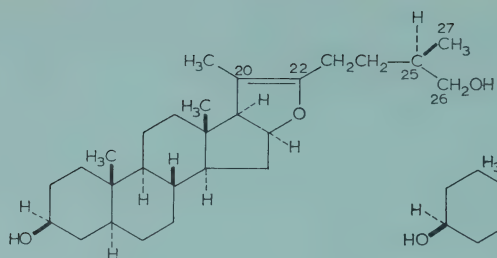


(55)
(20*R*,22*R*,25*R*)-5α-Spirostan
(Cyclopseudoisogenin*)



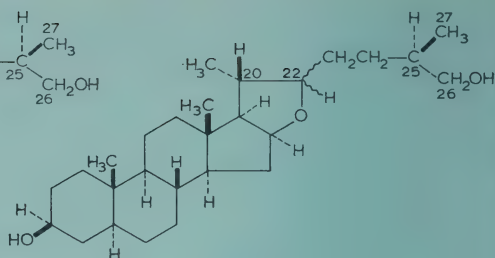
(56)
(20*S*,22ξ,25*S*)-5α-Furostan-26-ol
(Dihydrogenin*)

* The standard name is preferred.



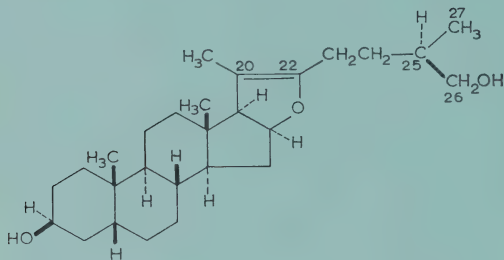
(57)

(25*R*)-5α-Furost-20(22)-en-3β,26-diol
(Pseudotigogenin*)



(58)

(20*S*,22ξ,25*R*)-5α-Furostan-3β,26-diol
(Dihydropseudotigogenin*)



(59)

(25*S*)-5β-Furost-20(22)-en-3β,26-diol
(Pseudosarsasapogenin*)

Derivatives

Rule 2S-4 (extended version of Rule S-4)

4.1. Steroid derivatives that can be considered to be formed by modification of, or introduction of substituents into, a parent compound are named by the usual methods of organic chemistry (see *IUPAC Nomenclature of Organic Chemistry, Sections A and B* (1957), also *J. Am. Chem. Soc.*, 82 (1960) 5545, and *Section C* (1965), Butterworths, London, also *Pure Appl. Chem.*, 11, No. 1 and 2 (1965)).

Notes: For the benefit of the specialist, those rules of general substitutive nomenclature that apply most often to steroids are outlined here. For full detail the IUPAC Rules cited above should be consulted.

I. Unsaturation is indicated by changing terminal “-ane” to “-ene”, “-adiene”, “-yne”, etc., or “-an” to “-en”, “-adien”, “-yn”, etc.; e.g., 5α-cholest-6-ene, 5β-cholesta-7,9(11)-diene, 5-spirosten: see also the names of Examples (22)–(25)**.

II. Most substituents can be designated either as suffixes or as prefixes; a few can be named only as prefixes, the commonest of these being halogens, alkyl, and nitro groups. When possible, one type of substituent must be designated as suffix. When more than one type is present that could be designated as suffix, one type only may be so expressed and the other types must be designated as prefixes.

* The standard name is preferred.

** For uniformity with the IUPAC Rules cited above, the conventions of *Chemical Abstracts* are used also in the present Rules for the position of locants (positional numerals) and designation of unsaturation. In such matters, and in use of Δ to designate unsaturation (which is not recommended by IUPAC), authors should respect the house customs of the journals to which their papers are submitted.

Choice for suffix is made according to an order of preference that is laid down in the Rules cited above; the most important part of this order, for steroids, is as follows, in decreasing preference: 'onium salt, acid, lactone, ester, aldehyde, ketone, alcohol, amine, ether. Suffixes are added to the name of the saturated or unsaturated parent system, the terminal "e" of "-ane", "-ene", "-yne", "-adiene", *etc.*, being elided before a vowel (presence or absence of numerals has no effect on such elisions). The following examples illustrate the use of these principles.

(a) *Acids*. Suffix for $\text{—CH}_3 \rightarrow \text{—COOH}$: -oic acid.

Suffix for $\text{CH} \rightarrow \text{C—COOH}$: -carboxylic acid.

Examples:

11-Oxo-5 α -cholan-24-oic acid

(20S)-3 α -Hydroxy-5-pregnene-20-carboxylic acid

(b) *Lactones, other than cardanolides and bufanolides*. The ending "-ic acid" or "-carboxylic acid" of the name of the hydroxy acid is changed to "-lactone" or "-carbolactone", respectively, preceded by the locant of the acid group and then the locant of the hydroxyl group, and the prefix "hydroxy" is omitted for the lactonized hydroxyl group.

Examples:

3 β -Hydroxy-5 α -cholano-24,17 α -lactone

(20R)-3 β -Hydroxy-5-pregnene-20,18-carbolactone

(c) *Cardanolides and bufanolides*. The -olide ending of these names denotes the lactone grouping, and substituents must be named as prefixes.

(d) *Esters of steroid alcohols*. Special procedures are used. For esters of monohydric steroid alcohols, the steroid hydrocarbon radical name is followed by that of the acyloxy group in its anionic form. The steroid radical name is formed by replacing the terminal "e" of the hydrocarbon name by "yl" and inserting before this the locant and Greek letter, with hyphens, to designate the position and configuration.

Example:

5 α -Cholestan-3 β -yl acetate

For esters of polyols the name of the polyol (*cf.* (g) below) is followed by that of the acyloxy group(s) in its anionic form, with locants when necessary.

Examples:

5 β -Cholestane-3 α ,12 α -diol diacetate

5 β -Cholestane-3 α ,12 α -diol 3-acetate 12-benzoate

Estradiol-17 β 17-monoacetate

When an acid, lactone, or spirostan group is also present, the ester group is designated by an acyloxy prefix.

Example:

(25S)-3 β -Acetoxy-5 β -spirostan

(e) *Aldehydes*. Suffixes: -al (denotes change of —CH_3 to —CHO , *i.e.*, without change in the number of carbon atoms); -aldehyde (denotes change of —COOH to —CHO , *i.e.*, without change in the number of carbon atoms; name derived from that of the acid).

Prefix: oxo- (denotes change of $>\text{CH}_2$ to $>\text{CO}$, thus also of $-\text{CH}_3$ to $-\text{CHO}$, with no change in the number of carbon atoms).

Examples:

5 α -Androstan-19-al
5 α -Cholan-24-aldehyde
19-Oxo-5 α ,17(α H)-etianic acid

Other methods are used for introduction of additional carbon atoms as $-\text{CHO}$ groups.

(f) *Ketones*: Suffix: -one.

Prefix: oxo-.

Examples:

5 β -Androstan-3-one
5-Pregnene-3,20-dione
11-Oxo-5 α -cholan-24-oic acid

(g) *Alcohols*. Suffix: -ol.

Prefix: hydroxy-

Examples:

5 β -Cholestane-3 α ,11 β -diol
3 α -Hydroxy-5 α -androstan-17-one

Notes: (1) Composite suffixes -olone and -onol, to denote simultaneous presence of hydroxyl and ketonic groups, are not permitted by IUPAC Rules and should not be used. (2) A few trivial names exist for hydroxy ketones, such as testosterone for 17 β -hydroxy-4-androsten-3-one (see Rule 2S-4.2).

(h) *Amines*. Suffix: -amine.

Prefix: amino-.

The suffix may be attached to the name of the parent compound or of its radical.

Examples:

5-Androsten-3 β -amine or 5-Androsten-3 β -ylamine
3 β -(Dimethylamino)-5 α -pregnan-20 α -ol

(i) *Ethers*. Ethers are named as alkoxy derivatives when another group is present that has priority for citation as suffix.

Examples:

3 β -Ethoxy-5 α -cholan-24-oic acid
17 β -Methoxy-4-androsten-3-one

When no such other group is present, ethers of steroid monoalcohols may be named by stating the name of the steroid hydrocarbon radical, followed by the name of the alkyl (or aryl, *etc.*) radical, and lastly by "ether"; in English these three parts of the name are printed as separate words, for example, 5 α -androstan-3 β -yl methyl ether. For ethers of steroid polyols the same system may be used but with the name of the steroid hydrocarbon radical replaced by the name of the polyol; for partially etherified polyols, locant(s) precede the names of the alkyl (or aryl, *etc.*) group(s); for example, 5 α -pregnane-3 β ,17 α ,20 α -triol trimethyl ether, 5 α -pregnane-3 β ,17 α ,20 α -triol 3,17-dimethyl ether, cortisol 21-methyl ether.

4.2. The following are examples of trivial names retained for important steroid derivatives, these being mostly natural compounds of significant biological activity:

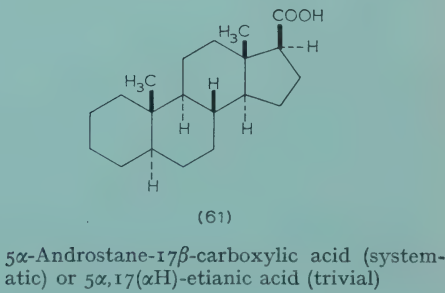
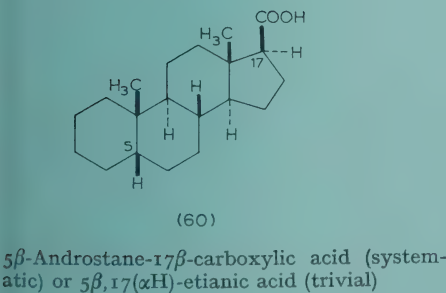
Alosterone	18,11-Hemiacetal of 11 β ,21-dihydroxy-3,20-dioxo-4-pregnen-18-al
Androsterone	3 α -Hydroxy-5 α -androstan-17-one
Cholecalciferol*	9,10-Seco-5,7,10(19)-cholestatrien-3 β -ol (for seco see Rule 2S-8)
Cholesterol	5-Cholesten-3 β -ol
Cholic acid	3 α ,7 α ,12 α -Trihydroxy-5 β -cholan-24-oic acid
Corticosterone	11 β ,21-Dihydroxy-4-pregnene-3,20-dione
Cortisol	11 β ,17 α ,21-Trihydroxy-4-pregnene-3,20-dione
Cortisol acetate	Cortisol 21-acetate
Cortisone	17 α ,21-Dihydroxy-4-pregnene-3,11,20-trione
Cortisone acetate	Cortisone 21-acetate
Deoxycorticosterone	21-Hydroxy-4-pregnene-3,20-dione (<i>i.e.</i> , the 11-deoxy derivative of corticosterone)
Ergocalciferol*	9,10-Seco-5,7,10(19),22-ergostatetraen-3 β -ol (for seco see Rule 2S-8)
Ergosterol	5,7,22-Ergostatrien-3 β -ol
Estradiol-17 α	1,3,5(10)-Estratriene-3,17 α -diol
Estradiol-17 β	1,3,5(10)-Estratriene-3,17 β -diol
Estriol	1,3,5(10)-Estratriene-3,16 α ,17 β -triol
Estrone	3-Hydroxy-1,3,5(10)-estratrien-17-one
Lanosterol	8,24-Lanostadien-3 β -ol
Lithocholic acid	3 α -Hydroxy-5 β -cholan-24-oic acid
Progesterone	4-Pregnene-3,20-dione
Testosterone	17 β -Hydroxy-4-androsten-3-one

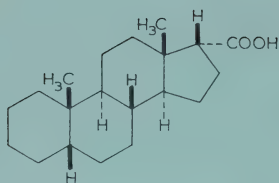
* Included in the List of Trivial Names for Miscellaneous Compounds of Biochemical Importance published by the IUPAC-IUB Commission of Biochemical Nomenclature; see, for example, *IUPAC Inform. Bull.*, 25 (1966) 19, or *J. Biol. Chem.*, 241 (1966) 2987, or *Biochim. Biophys. Acta*, 107 (1965) 1.

Note: If these trivial names are used as a basis for naming derivatives or stereoisomers, the derived trivial name must make the nature of the modification completely clear and is preferably accompanied at first mention by the full systematic name. For example, in steroid papers “epi” is often used with trivial names to denote inversion at one centre; the name “11-epicortisol” defines the compound fully since cortisol is already defined as the 11 β -alcohol; but the name “epicortisol” does not define the compound and is inadequate.

4.3. Androstane-17-carboxylic acids may be called “etianic acids”, although the former (systematic) name is preferred. The orientation of the hydrogen atoms at positions 5 and 17 must in all cases be indicated as 5 α or 5 β , and 17(α H) or 17(β H), respectively.

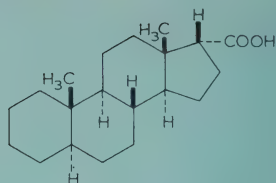
Examples:





(62)

5β-Androstane-17α-carboxylic acid (systematic) or 5β,17(βH)-etianic acid (trivial)



(63)

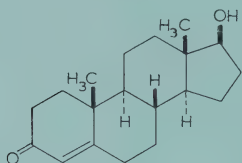
5α-Androstane-17α-carboxylic acid (systematic) or 5α,17(βH)-etianic acid (trivial)

Stereochemical modifications

Rule 2S-5 (extended version of Rule S-5)

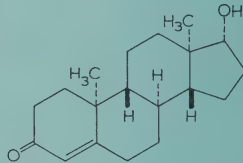
5.1. If, as for instance in a synthetic compound, there is stereochemical inversion at all the asymmetric centres whose configurations do not require to be specified in a name, the italicized prefix *ent*- (a contracted form of *enantio*-) is placed in front of the complete name of the compound. This prefix denotes inversion at all asymmetric centres (including those due to named substituents) whether these are cited separately or are implied in the name.

Examples:



(64)

17β-Hydroxy-4-androsten-3-one
(Testosterone)



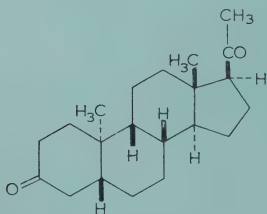
(65)

ent-17β-Hydroxy-4-androsten-3-one
(*ent*-Testosterone)

Note: When Roman or Arabic numerals are used to enumerate formulae, the prefix *ent*- may be used to indicate the enantiomer. Thus, *e.g.*, (65) above may be designated (*ent*-64).

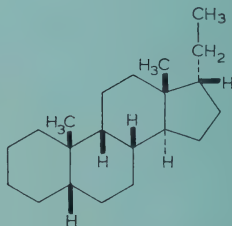
5.2. If there is stereochemical inversion at a minority of the asymmetric centres whose configurations do not require to be specified in a name, the configuration of the hydrogen atoms or substituents at the affected bridgeheads, or the carbon chain (if any) at position 17, are stated by means of a prefix or prefixes α or β, each with its appropriate positional numeral, placed before the stem name laid down in the preceding Rules.

Examples:



(66)

5β,9β,10α-Pregnane-3,20-dione



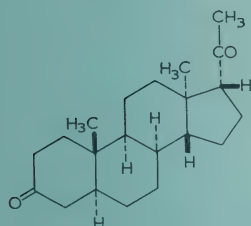
(67)

5β,9β,17α-Pregnane

5.3. The enantiomer of a compound designated as in Rule 5.2 is given the same name preceded by *ent*-.

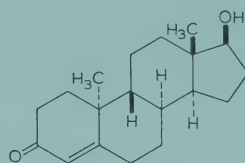
Note: This Rule covers the compounds in which there is inversion at a majority but not all, of the asymmetric centres that do not require to be specified in the name.

Examples:



(68) = (*ent*-66)

ent-5 β ,9 β ,10 α -Pregnane-3,20-dione
(not 5 α ,8 α ,13 α ,14 β ,17 α -pregnane-3,20-dione)

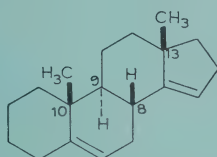


(69)

ent-17 α -Hydroxy-13 α ,14 β -androst-4-en-3-one
(not 17 β -hydroxy-8 α ,9 β ,10 α -androst-4-en-3-one)

5.4. If there is stereochemical inversion at half of the asymmetric centres whose configurations are implied in the stem name of a "normal" steroid (*e.g.*, 70), the prefixes to be specified in the name of the stereoisomer are that set that includes the number occurring first in the series 8, 9, 10, 13, 14, 17 without or with the prefix *ent*- as appropriate.

(70)
"Normal" steroid



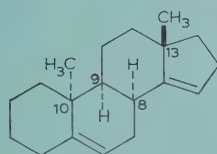
Configuration at
asymmetric centres

Name

8 β ,9 α ,10 β ,13 β

5,14-An-
drostadiene

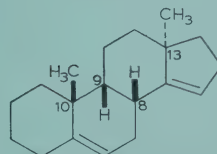
(71)
Steroid inverted at
8 and 10; "normal"
at 9 and 13



8 α ,9 α ,10 α ,13 β

8 α ,10 α -
Androsta-
5,14-diene

(72) (*ent*-71)
Steroid inverted at
9 and 13; "normal"
at 8 and 10



8 β ,9 β ,10 β ,13 α

ent-8 α ,10 α -
Androsta-
5,14-diene

Note: (72) could also logically be named "9 β ,13 α -androsta-5,14-diene"; this name might seem simpler, but it has the disadvantage that it does not indicate that (72) is the enantiomer of (71).

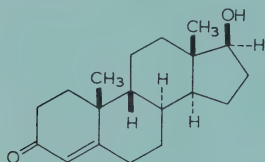
5.5. Racemates, as for instance obtained by synthesis, are named by use of an italicized prefix *rac*- (an abbreviation of *racemo*-), placed before the complete name of the compound, the enantiomer chosen for naming being that required by Rules 2S-5.1 to 2S-5.4.

Example: A racemate composed of (64) and (65) (= *ent*-64) is named:

rac-17 β -Hydroxy-4-androsten-3-one or *rac*-testosterone

5.6. (a) When the relative, but not the absolute, configuration of two or more asymmetric centres in a steroid derivative is known, as for instance for a compound obtained by synthesis, the 10 β configuration is taken as basis for the name; or, if C-10 is not asymmetric or is absent, the lowest-numbered asymmetric bridgehead is designated α (or *R*); the other asymmetric centres are then considered as α or β (or *R* or *S*) relative to that one; and the whole name is prefixed by *rel*- (italicized). Individual asymmetric centres may be referred to as α^* , β^* , R^* , or S^* (spoken as alpha star, R star, *etc.*) but these symbols are not used in the name of the compound.

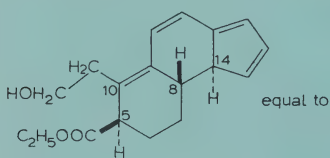
(b) When both enantiomers of known relative, but unknown absolute, configuration are prepared, they are distinguished by a prefix (+)-*rel*- or (–)-*rel*-, where the *plus* or *minus* sign refers to the direction of rotation of plane-polarized light (the wavelength, solvent, temperature and/or concentration must be added when known to affect this sign).



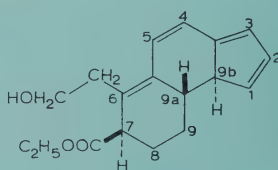
(73)

The dextrorotatory form having either this or the enantiomeric configuration would be named:

(+)-*rel*-17 β -Hydroxy-8 α ,9 β -androst-4-en-3-one



(74A)



(74B)

(74A) *rel*-(Ethyl 2-hydroxy-2,3-seco-*A*-nor-5 α -gona-9,11,13(17),15-tetraen-3-oate)

(for seco see Rule 2S-8 and for nor see Rule 2S-7)

or (74B) *rel*-[(7*R*,9*aS*,9*bS*)-Ethyl 8,9,9*a*,9*b*-tetrahydro-7*H*-cyclopenta[*a*]naphthalene-7-carboxylate]

Note: At some stage in synthetic work on steroids, names of intermediates have to be changed from a system used in general organic chemistry to the steroid system. The names (74A) and (74B) illustrate such a change and it should be noted (i) that not merely the name but also the numbering are usually changed and (ii) that the steroid name usually avoids the need to specify the configuration at each asymmetric centre. The latter factor will often indicate at what point in a synthesis the change of nomenclature is desirable.

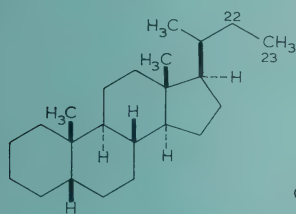
Shortening of side chains and elimination of methyl groups

Rule 2S-6 (expanded from Rule S-6)

6.1. Elimination of a methylene group from a steroid side chain (including a

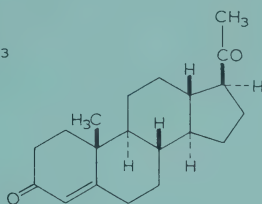
methyl group) is indicated by the prefix "nor-", which in all cases is preceded by the number of the carbon atom that disappears. When alternatives are possible, the number attached to nor is the highest permissible. Elimination of two methylene groups is indicated by the prefix "dinor-".

Examples:



(75)

24-Nor-5β-cholane



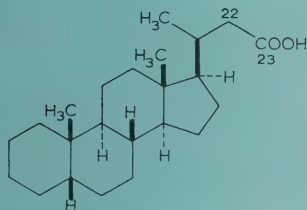
(76)

18-Nor-4-pregnene-3,20-dione

Exceptions: By Rules 2S-2.1 and 2S-2.2 the names gonane (for 18,19-dinorandrostane) and estrane (for 19-norandrostane) constitute exceptions to the above Rule 2S-6.1. The names gonane and estrane are used also as parent names for their derivatives.

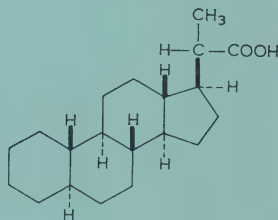
However, 18-nor- and 19-nor- are used with other trivial names, as in 19-norpregnane, 18,19-dinorspirostan, 18-norestrone.

The compound produced by shortening the 17-side chain of pregnane is named 17-methylandrosterane rather than 21-norpregnane. See also Note to Rule 2S-2.2.



(77)

24-Nor-5β-cholan-23-oic acid



(77a)

18,19-Dinor-5α-pregnane-20α-carboxylic acid

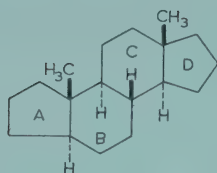
Ring contraction or expansion

Rule 2S-7 (amended version of Rule S-7)

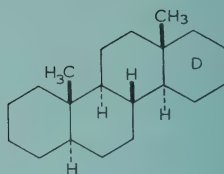
7.1. Ring contraction and ring expansion (other than insertion of atoms between directly linked bridgeheads or, when a steroid side chain is present, between C-13 and C-17) are indicated by prefixes "nor" and "homo", respectively, preceded by an italic letter indicating the ring affected. For loss or insertion of two methylene groups, "dinor" and "dihomo" are used. "Homo" and "nor", when occurring in the same name, are cited in alphabetical order*.

* Alphabetical order is used for any combination of cyclo, homo, nor, and seco; they are placed immediately before the stem name and after any prefixes denoting substituents.

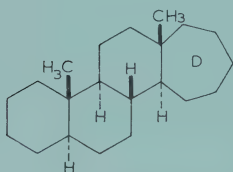
Examples:



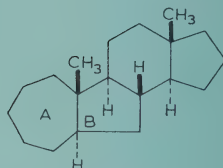
(78)

A-Nor-5 α -androstane

(79)

D-Homo-5 α -androstane

(80)

D-Dihomo-5 α -androstane

(81)

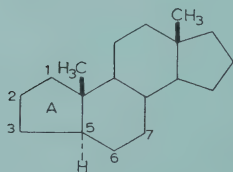
A-Homo-*B*-nor-5 α -androstane

Notes: (a) By too extended use, this nomenclature can be applied to compounds whose steroid character is excessively modified. It is recommended that it be confined to steroids containing at least one angular methyl group, or a steroid C_{17} -side chain, or a steroidal group on ring *D* (e.g., a spirostan); also that no more than two of the steroid rings may be altered by any combination of the operations denoted by “nor” and “homo”. When these conditions are not met, general systematic nomenclature should be used.

(b) Names incorporating “homo” and “nor” are normally preferred to alternatives incorporating “cyclo” and “seco” (cf. Example (86)).

7.2. On ring contraction the original steroid numbering is retained, and only the highest number(s) of the contracted ring, exclusive of ring junctions, is deleted.

Example:

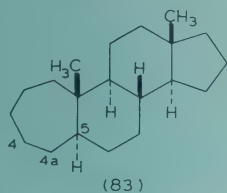


(82)

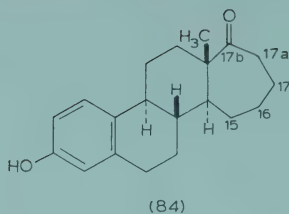
A-Nor-5 α -androstane (Number 4 is omitted)

7.3. On ring expansion (other than insertion of atoms between directly linked bridgeheads or, when a C_{17} -side chain is present, between C_{13} and C_{17}), the letter *a* (and *b*, etc., as necessary) is added to the highest number in the ring enlarged exclusive of ring junctions, and this letter and number are assigned to the last peripheral carbon atom in the order of numbering of the ring affected.

Examples:



A-Homo-5 α -androstane

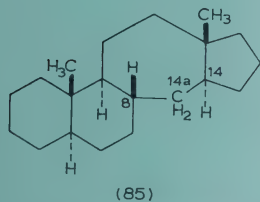


3-Hydroxy-D-dihomo-1,3,5(10)-estratrien-17b-one

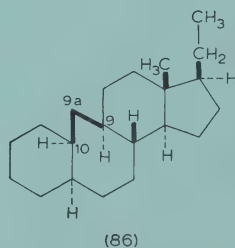
7.4. Ring expansion by formal insertion of a methylene group between directly linked bridgeheads is indicated as shown in the annexed table. The italic capital letters denote the ring(s) affected; the locants in parentheses (which are included in the name) are those of the inserted methylene groups.

<i>CH₂ added between</i>	<i>Prefix used</i>
C-5 and C-10	<i>AB(10a)-Homo</i>
C-8 and C-9	<i>BC(8a)-Homo</i>
C-8 and C-14	<i>C(14a)-Homo</i>
C-9 and C-10	<i>B(9a)-Homo</i>
C-13 and C-14	<i>CD(13a)-Homo</i>

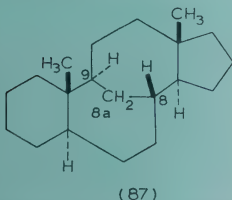
Examples:



C(14a)-Homo-5 α -androstane



*B(9a)-Homo-19-nor-5 α ,10 α (H)-pregnane**



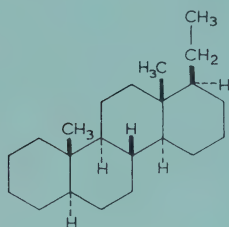
BC(8a)-Homo-5 α -androstane

7.5. Expansion of ring *D* by insertion of atoms between C-13 and C-17: The names "*D*-homopregnane", "*D*-homocholane", etc., are used only for the isomer with the side chain at position 17a (*cf.* Example (88)). Isomers with the side chain at

* This name is preferred to 9 β ,19-cyclo-9,10-seco-5 α ,10(α H)-pregnane (see Note b to Rule 2S-7.1). This skeleton is contained in some *Buxus* alkaloids.

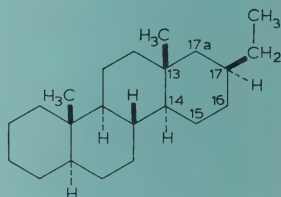
position 17 (formed by formal insertion of a methylene group between C-13 and C-17) are named as derivatives of androstane, estrane, or gonane (*cf.* Example (89)). As exceptions, furostans and spirostans into which a methylene group has been formally inserted between C-13 and C-17 are given these names with an added prefix "*D*(17*a*)-homo" (*cf.* Example (90)).

Examples:



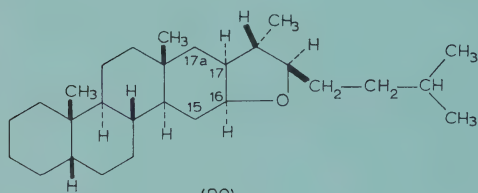
(88)

D-Homo-5 α -pregnane



(89)

17 β -Ethyl-*D*-homo-5 α -androstane



(90)

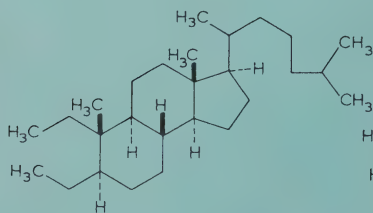
(22*R*)-*D*(17*a*)-Homo-5 β -furostan

Ring fission

Rule 2S-8 (unchanged from Rule S-7.4)

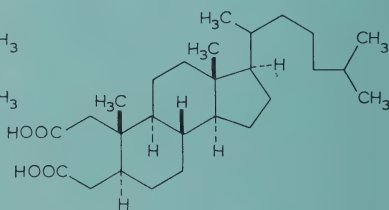
8.1. Fission of a ring, with addition of a hydrogen atom at each terminal group thus created, is indicated by the prefix "*seco*-", the original steroid numbering being retained*.

Examples:



(91)

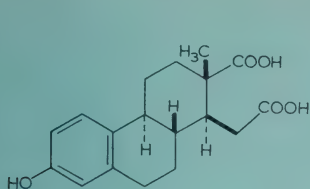
2,3-Seco-5 α -cholestane



(92)

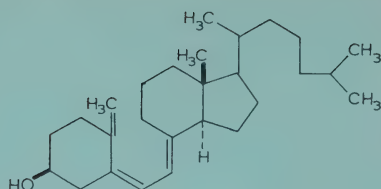
2,3-Seco-5 α -cholestane-2,3-dioic acid

* If more than one ring is opened, general systematic nomenclature may be preferable. The principles of Note a to Rule 2S-7.1 apply also to *seco*-steroids.



(93)

3-Hydroxy-16,17-seco-1,3,5(10)-estratriene-16,17-dioic acid



(94)

9,10-Seco-5,7,10(19)-cholestatrien-3 β -ol
(trivial name: cholecalciferol*)

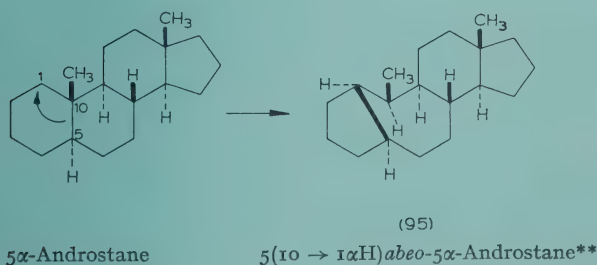
Modification by bond migration (*abeo* system)

Rule 2S-9 (new)

9.1. A compound that does not possess a steroid skeleton but may be considered formally to arise from a steroid by bond migration may be given the name laid down in the preceding Rules for the steroid in question, to which is attached a prefix of the form $x(y \rightarrow z)$ *abeo*-. This prefix is compiled as follows: A numeral denoting the stationary (unchanged) end of the migrating bond (x) is followed by parentheses enclosing (i) the number denoting the original position (y) from which the other end of this bond has migrated, (ii) an arrow, and (iii) the number (z) denoting the new position to which the bond has moved. The closing parenthesis is followed by *abeo*- (Latin, I go away) (italicized) to indicate bond migration. The original steroid numbering is retained for the new compound and is used for the numbers x , y , and z . Such of the customary letters as are necessary are added to specify the resulting stereochemistry.

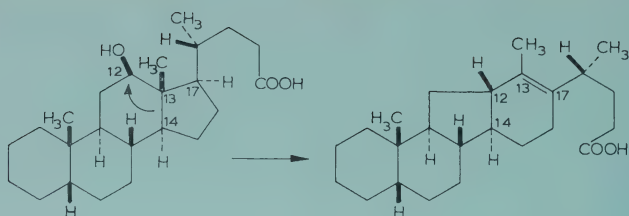
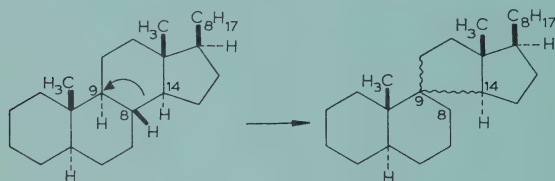
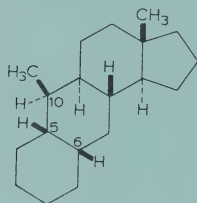
Note: The *abeo* nomenclature described in this Rule is permissive, not compulsory. It is most suitable for use in discussions of reaction mechanism and biogenesis. For registration in a general (non-steroid) compendium the general systematic names may be preferable, particularly when names of steroid type can be conveniently assigned by the homo-nor method. Differences in numbering between *abeo* names and other systematic names should be particularly noted (*cf.* Example (96)).

Examples:



* This trivial name is retained (see Rule 2S-4.2).

** Name according to Rule 2S-7.4: 9 β -Methyl-*B*(9 α)-homo-*A*-nor-5 α , 10 α -estrane.

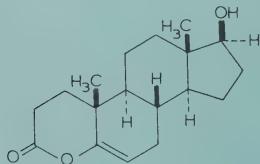
12 β -Hydroxy-5 β -cholan-24-oic acid(96)
14(13 \rightarrow 12 β H)abeo-5 β -Chol-13(17)-en-24-oic acid*5 α -Cholestane(97)
14(8 \rightarrow 9 ξ)abeo-5 α -Cholestane**

(98)

1(10 \rightarrow 6 β H)abeo-5 β -Androstane (an anthrasteroid)*Hetero modifications**Rule 2S-10* (unchanged from Rule S-7.5)

10.1. If hetero atoms occur in the ring system of a steroid the replacement ("oxa-aza") system of nomenclature is used with steroid names and numbering (*cf.* IUPAC Rule B-4; also Introduction to IUPAC Rules C-o.6, the reference to IUPAC Rules C is given on p. 468).

Example:



(99)

17 β -Hydroxy-4-oxa-5-androsten-3-one

* Name according to Rules 2S-2.4 and 2S-8.1:
12 α ,14 β -Cyclo-13,14-seco-5 β -chol-13(17)-en-24-oic acid.

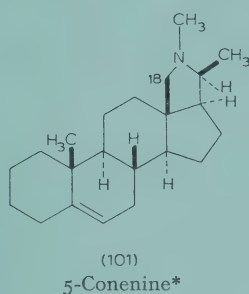
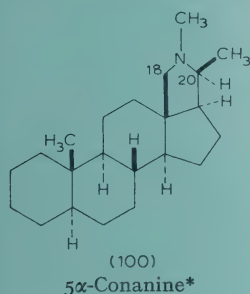
** The configuration at C-9, if known, is assigned by the sequence-rule procedure (for reference see footnote on p. 454).

Steroid alkaloids

Rule 2S-II (new)

11.1. When readily possible, systematic names for steroid alkaloids are derived from pregnane or some other steroid parent name. Trivial names for other steroid alkaloids are chosen so that the name for the saturated system ends in “-anine”. In names for unsaturated compounds this ending is changed to “-enine”, “-adienine”, etc., as appropriate. When asymmetry exists at positions 8, 9, 10, 13, 14, 16, 17, 20, or, 23, it is implied in the name, as set out in the annexed table and formulae, and divergences are designated as laid down in Rule 2S-5. Configurations at positions 5, 22, and 25 must be specified with the name. Sequence-rule symbols are used for positions numbered 20 or higher.

Examples: Typical examples of parent names for groups of alkaloids are given in the following table and the corresponding formulae. It must be noted that substitution or unsaturation may alter the *R,S* designations for derivatives.

PARENT NAMES FOR GROUPS OF STEROID ALKALOID^a

Formula	Name of parent	Stereochemistry ^b implied in the name, as shown in the formula	Stereochemistry to be indicated by sequence-rule prefixes (or ξ)
100	Conanine	17 α H, 20S	—
102	Tomatanine ^c	16 α H, 17 α H, 20S	22, 25
103	Solanidanine ^d	16 α H, 17 α H, 20S	22, 25
104	Cevanine ^e	17 α H, 13 β H, 20R	22, 25
105	Veratranine ^{e,f}	17 α H, 20S	22, 25
106	Jervanine ^{e,f}	17 α O, 20R	22, 23, 25

^a Some of the names in this table were suggested in the Introduction to *Optical Rotatory Power*, 1a, *Steroids*, Tables des Constantes, Pergamon Press, Oxford, 1965, p. 2a and 2f.

^b Additional to that at positions 8, 9, 10, 13, and 14.

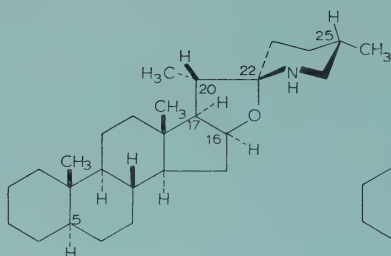
^c The compounds are oxa-aza analogues of the spirostans (which are dioxo spiro compounds). Formulae are conveniently drawn analogously to those of the spirostans.

^d This group includes rubijervine and isorubijervine.

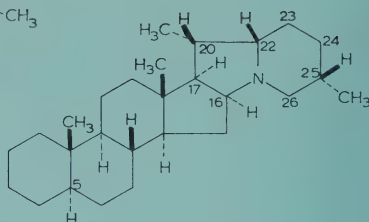
^e These structures contain a *D*-homo-*C*-nor skeleton, with the stereochemistry shown. However, they are commonly considered as 14(13 \rightarrow 12)*abeo* structures and are numbered as such.

^f Jervanine, as defined here, is the same as veratranine except for addition of an epoxy bridge, but it is convenient to have two separate names: the veratranine skeleton (see 105) is present in the alkaloid veratramine. It should be noted that the name 5 α -jervane has been used for the rearranged hydrocarbon skeleton (107) (J. FRIED AND A. KLINGSBERG, *J. Am. Chem. Soc.*, 75 (1953) 4934), for which the *abeo*-type numbering given in (107) is here recommended.

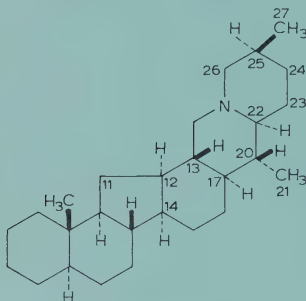
* Cf. R. D. HAWORTH AND M. MICHAEL, *J. Chem. Soc.*, (1957) 4973.



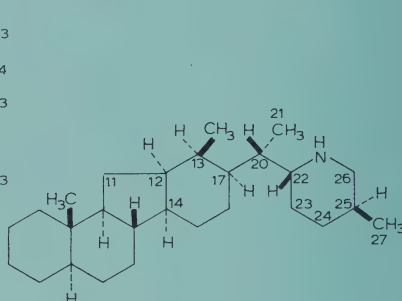
(102)

(22*S*,25*S*)-5α-Tomatanine

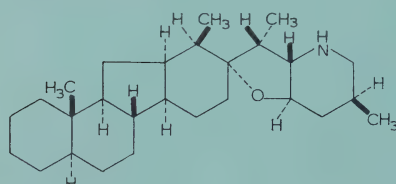
(103)

(22*S*,25*S*)-5α-Solanidanine

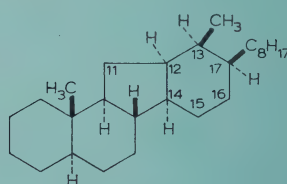
(104)

(22*S*,25*S*)-5α-Cevanine

(105)

(22*R*,25*S*)-5α-Veratranine

(106)

(22*S*,23*R*,25*S*)-5α-Jervanine

(107)

5α-Jervane*

APPENDIX

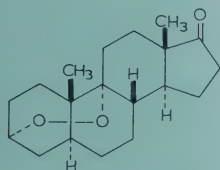
Guide lines for steroids containing additional rings

I. *General.* When additional rings are formed within, or on, a steroid nucleus, situations often arise where either the resemblance to a normal steroid is obscured or the steroid-type name becomes so complex that recourse to general systematic nomenclature is preferable. On the other hand, the general rules, with one exception, are based on that form of each component that contains the maximum number of conjugated double bonds, the whole fused system is then renumbered, and the stereochemistry must be defined separately for each chiral position; the final name resulting is then cumbersome and in a form that is often barely recognizable by a steroid specialist chemist and even less so by a biochemist or biologist. The paragraphs below give suggestions as to how general nomenclature may be modified to

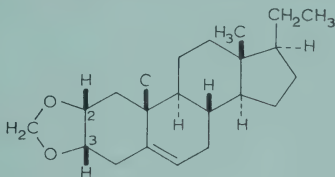
* Cf. J. FRIED AND A. KLINGSBERG, *J. Am. Chem. Soc.*, 75(1953) 4934.

incorporate steroid names, but without an attempt to legislate rigidly or to cover every case. The decision whether any one compound shall receive such a modified steroid name or a general systematic name is left to authors and editors in the particular circumstances of each case. Nor are the requirements of journals and compendia or abstracts necessarily identical.

2. *Rings derived from functional groups.* Bivalent functional groups such as $-O-$ and $-O-O-$ linked to two different positions, thus forming additional rings, are named by the ordinary methods of organic chemistry; for example, (108) is 3 α ,9-epidioxy-5 α -androstan-17-one. Similarly, methylenedioxy derivatives are best named as such, e.g., (109) 2 α ,3 α -methylenedioxy-5-pregnene. In the same way,



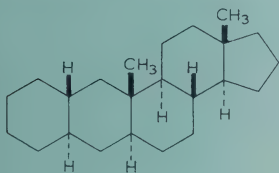
(108)



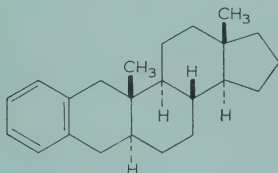
(109)

lactones and acetals formed by linkage between two different positions of a steroid skeleton are best named as such instead of by framing the name on the newly modified ring system.

3. *Additional carbocyclic or heterocyclic fused rings.* It is tempting to adapt the simple substitutive procedure for fusion of steroid nuclei with simple carbocyclic rings, particularly if the latter are saturated. Thus (110) might be named 2 α ,3 β -tetramethylene-5 α -androstan*. However, formation of additional rings by alkylene



(110)



(111)

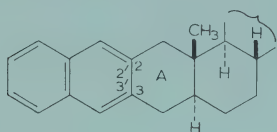
($-[CH_2]_x-$) prefixes is not in accord with IUPAC nomenclature and is often difficult to apply when unsaturation is present. Alternatives are thus preferable.

The exceptional case (Rule A-23.5) referred to above enables 2,3-benz-5 α -androst-2-ene to be a name for (111), and a slight extension of the rule would allow (110) to be called 2 β ,3 α -cyclohexano-5 α -androstan. Such methods might be used in simple cases but these too become difficult when complex ring systems are fused and often when unsaturation is present in the additional component.

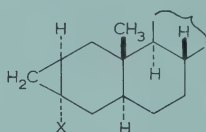
For a general procedure it is better to modify systematic IUPAC general practice to permit the steroid component to be cited in a reduced state, the reason why modification is necessary at all being of course the wish to keep the description of the stereochemistry as simple as possible. The suggestions below are closely similar to present practices of *Chemical Abstracts*.

* For simplicity, nomenclature in this Appendix is mostly described in terms of androstane, and partial formulae are to be understood accordingly. The principles, however, are general.

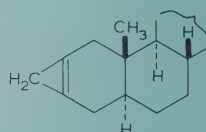
An additional carbocyclic component is cited in its most unsaturated form by its fusion name (usually ending in -o), placed in front of the name of the steroid component, and the position of fusion is indicated by numerals in square brackets; for instance, benz[2,3]-5 α -androst-2-ene for (111). Here note that the unsaturation of the benzo ring causes unsaturation also in the steroid component and this must be cited (-2-ene). Similarly, (112) is naphtha[2',3':2,3]-5 α -androst-2-ene; the steroid A ring is still considered unsaturated even though it may be preferred to write the



(112)



(113)



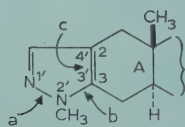
(114)

naphthalene double bonds as in the formula shown; note also that the locants for the non-steroid component receive primes, and that, when choice is possible, its locants for ring fusion are as low as possible and in the same direction as in the steroid component (*i.e.*, not 6',7':2,3 or 3',2':2,3).

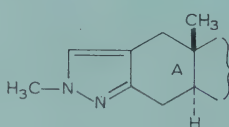
The reduced compound (110) is then 2 β ,3 α ,3',4',5',6'-hexahydrobenz[2,3]-5 α -androstane. Note the citation of the configuration at the new ring junction positions and that the steroid component is now cited in its saturated state.

Two further points can be illustrated with (113). Consider first the hydrocarbon where X = H. The additional ring is cited as cyclopropa, denoting an unsaturated three-membered ring as in (114). In (114) the position of the "extra" (indicated) hydrogen must be cited as 2'H. Reduction of (114) to (113; X = H) adds 2 α ,3 α -dihydro to the name, which thus becomes 2 α ,3 α -dihydro-2'H-cyclopropa[2,3]-5 α -androstane. If X were not hydrogen but, say, OH, the hydro prefixes would be still needed to show the state of hydrogenation and the OH group would be named additionally; in such cases it is preferable to state the configuration for the OH group that is present rather than that of the H atom that has been replaced; the name then becomes 2 α ,3-dihydro-2'H-cyclopropa[2,3]-5 α -androstan-3 α -ol.

The same fundamental principle can be used for heterocyclic components, but conveniently modified to accord with general nomenclature as follows: (a) the heterocyclic component is cited after the steroid component (to permit modification of the ending for salt formation, *etc.*), and (b) the position of fusion of the heterocyclic component is cited by letters as in the standard IUPAC and Ring Index method. Thus, (115) is 2'-methyl-2'H-5 α -androst-2-eno[3,2-c]pyrazole; note the numbering of the pyrazole ring so that numbers for ring fusion are as low as possible; if the



(115)

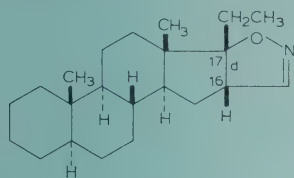


(116)

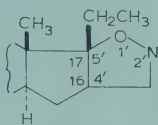
methyl group in (115) were replaced by hydrogen, the double bonds would be placed in the mesomeric pyrazole ring just as in (115) so as to retain this low numbering

for ring fusion. In the isomer (116) the steroid component is no longer unsaturated and is therefore cited as androstano-; the full name for (116) is 1'-methyl-1'*H*-5 α -androstano[3,2-*c*]pyrazole.

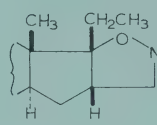
Further problems arise when ring fusion involves a quaternary carbon atom. The name for (117), for instance, could be built up as follows: to 5 α -pregnane is



(117)

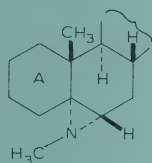


(118)

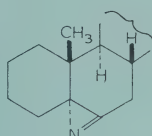


(119)

fused an isoxazole skeleton, giving (118); into this, only one double bond can be introduced, so that one hydrogen atom must be added as indicated hydrogen, which gives a 4' *β H*- prefix and a skeleton (119). The last step, inserting the double bond, gives the full name 4' *β H*-5 α -pregnano[16,17-*d*]isoxazole, even though it appears in (117) as if the heterocyclic ring should be named as the partly hydrogenated system isoxazoline.



(120)

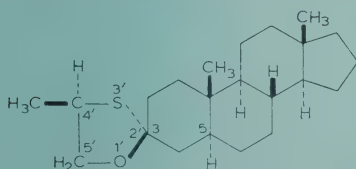


(121)

Not all such fusions cause all these complications. For instance, for (120) one fuses androstane to azirine, obtaining a skeleton into which one inserts a double bond as in the hypothetical compound (121); then, clearly, (120) is 1',3'-dihydro-1'-methyl-5 α -androstano[5,6-*b*]azirine.

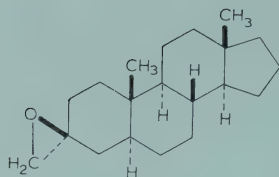
4. *Stereochemistry*. Stereochemistry in additional rings that lie in the approximate plane of rings A—D is cited as α or β , but in other cases by means of sequence-rule symbols.

5. *Spiro derivatives*. Spiro derivatives of steroids are named in accordance with the principles laid down in IUPAC Rules A-41, A-42, B-10, and B-11. Additional stereochemistry due to the spiro junction and substituents in the non-steroid ring is designated by the sequence-rule procedure. Alternative names permitted by IUPAC Rules are illustrated for (122) and (123).



(122)

4'*R*-Methyl-(*R*)-spiro[5 α -androstane-3,2'-(1',3'-oxathiolane)]
or 5 α -androstane-3(*R*)-spiro-2'-(4'*R*-methyl-1',3'-oxathiolane)



(123)

(3*S*)-Spiro[5α-androstane-3,2'-oxiran]
or (3*S*)-5α-androstane-3-spiro-2'-oxiran

OTHER TENTATIVE RULES OF THE IUPAC-IUB COMMISSION ON BIOCHEMICAL NOMENCLATURE ARE AS FOLLOWS:

Abbreviations and Symbols for Chemical Names of Special Interest in Biological Chemistry, J. Biol. Chem., 241 (1966) 527; Section 5 of this document (*Nucleotides and Nucleic Acids*) was also published in *Biochim. Biophys. Acta*, 108 (1965) 1.

Abbreviated Designation of Amino Acid Derivatives and Polypeptides, Biochim. Biophys. Acta, 121 (1966) 1.

Rules for Naming Synthetic Modifications of Natural Peptides, Biochim. Biophys. Acta, 133 (1967) 1.

Trivial Names of Miscellaneous Compounds of Importance in Biochemistry, Biochim. Biophys. Acta, 107 (1965) 1.

Nomenclature of Quinones with Isoprenoid Side-Chains, Biochim. Biophys. Acta, 107 (1965) 5.

Nomenclature and Symbols for Folic Acid and Related Compounds, Biochim. Biophys. Acta, 107 (1965) 11.

Nomenclature of Corrinoids, Biochim. Biophys. Acta, 117 (1966) 285.

The Nomenclature of Lipids, Biochim. Biophys. Acta, 152 (1968) 1.

Cyclitol Nomenclature, Biochim. Biophys. Acta, 165 (1968) 1.

Abbreviated Nomenclature of Synthetic Polypeptides (Polymerized Amino Acids), Biochim. Biophys. Acta, 168 (1968) 1.

A One-Letter Notation for Amino Acid Sequences, Biochim. Biophys. Acta, 168 (1968) 6.

Biochim. Biophys. Acta, 164 (1968) 453-486

TENTATIVE PROPOSALS FOR NOMENCLATURE* OF ABSOLUTE CONFIGURATIONS CONCERNED WITH SIX-COORDINATED COMPLEXES BASED ON THE OCTAHEDRON**

1. Introduction

1.1 Configuration

For spectroscopic purposes and for following the stereochemical course of substitution reactions it is of interest to consider, for example, tris- and bis-bidentate six-coordinated complexes based on the octahedron as related through the configurations depicted in Fig.1 (a) and (b). Here the edges spanned by the chelate rings are drawn as heavy lines. The chelate rings are thought of as devoid of chemical significance in the sense that the chelating ligands may be identical or different, and may be symmetrical or not. Similarly the two X's represent two monodentate ligands which may or may not be identical. It is desired, in all generality, to have a designation of chirality which is independent of the chemical nature of the chelating ligands and which only depends on the relative positions of the heavy line edges which represent the bidentate ligands or the bidentate units of polydentate ligands.

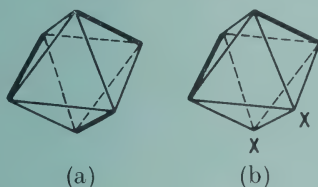


Fig. 1 General "octahedral" systems containing three (a) and two (b) bidentate ligands represented by the edges (drawn as heavy lines) which they span. It is desired to characterize these systems as having the same absolute configuration independently of their chemical significance. They have both been designated by Δ in the present proposal

1.2 Conformation

Further for spectroscopic purposes it is of interest to designate the conformation of chelate rings relative to the central atom or ion, but independently of the other atoms forming the chelate ring and also of the substituents of these atoms.

* The rules proposed here are given in short form in paragraph 8 and 9 of this communication

** Comments should be sent to the chairman of the Commission, Prof. K.A.JENSEN, Chemical Laboratory II of the University of Copenhagen, The H.C.Ørsted Institute, Universitetsparken 5, 2100 Copenhagen Ø

1.3 *The present proposals*

All the tentative rules which follow are based on the fact that two skew and non-orthogonal lines define a helical system. They primarily describe a nomenclature for the absolute configuration of classes comprising *cis*-bis-bidentate and tris-bidentate complexes and the absolute conformation of five-membered chelate rings. However, since the rules are based on general grounds, they lend themselves readily to application to more complicated situations, *i.e.* polydentate chelate systems and larger chelate rings.

In the chemical literature there exist different proposals for the nomenclature of the systems, devoid of chemical significance, which are under consideration here. These proposals are generally based upon helicities about symmetry or pseudo-symmetry axes. The present proposals are independent of symmetry concepts and thereby easier to generalize to situations where symmetry is absent.

2. **Basic principle**

Two skew lines which are not orthogonal to each other make up a helical system as illustrated in Fig. 2 and 3. Two skew lines possess the property of having one and only one normal in common. In Fig. 2 one of the skew

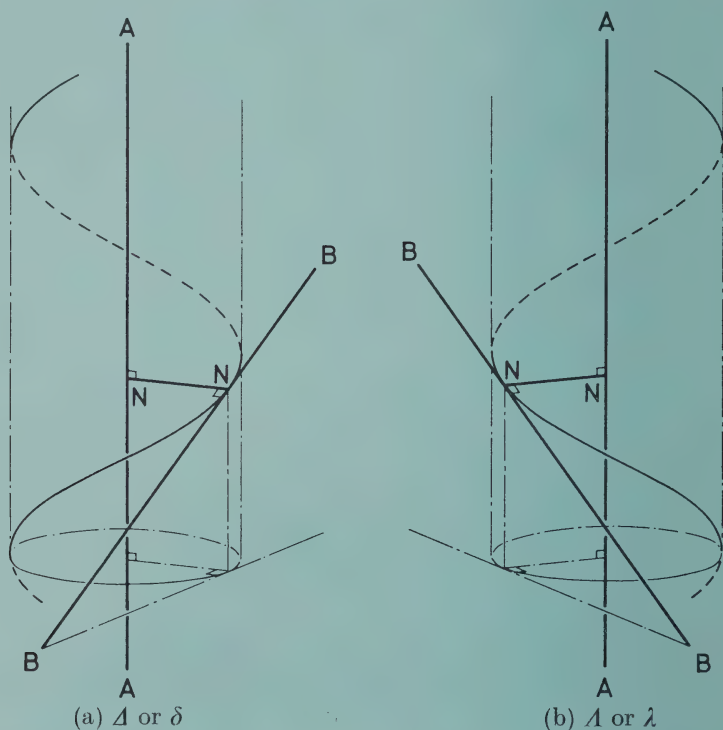


Fig. 2 Two skew lines AA and BB which are not orthogonal define a helical system. In the figure AA is taken as the axis of a cylinder whose radius is determined by the common normal NN of the two skew lines. The line BB is a tangent to the above cylinder at its crossing point with NN and defines a helix upon this cylinder by being the tangent to it at this crossing point. (a) and (b) illustrate a right- and a left-handed helix

lines AA determines the axis of a helix upon a cylinder whose radius is equal to the length of the two skew lines' common normal NN . The other of the skew lines BB makes up a tangent to the helix at N and determines the steepness of the helix. In Fig. 3 the two skew lines AA and BB are seen in projection on to a plane orthogonal to their common normal.

(a) of Fig. 2 and 3 illustrates a right-handed helix to be associated with the Greek letter delta (Δ referring to configuration, δ to conformation). (b) of Fig. 2 and 3 illustrates a left-handed helix to be associated with the Greek letter lambda (Λ for configuration, λ for conformation)*.

Because we are only interested in a qualitative measure of the helicity, the steepness of a helix is, in general, of no importance. However, the singularities at infinite steepness, where the skew lines become parallel lines, and at vanishing steepness, where the lines become orthogonal, should be noted. Here an infinitely small rotation of one line relative to the other about their common normal will change the helicity from right-handedness to left-handedness or vice versa. It is obvious that as the representation of our physical situation approaches these singularities the helicity becomes undefined (see Fig. 13).

3. Application to configuration

3.1 Representation to chelate rings

A chelate ring of a six-coordinated complex, whose ligators form an approximate octahedron, is represented by the edge determined by its two ligators. If two such edges are skew the pair can, without any further conventions, be associated** with either (a) or (b) of Fig. 3. This is the basis of the present proposal for nomenclature of absolute configurations.

Cis-bis-bidentate and tris-bidentate systems.

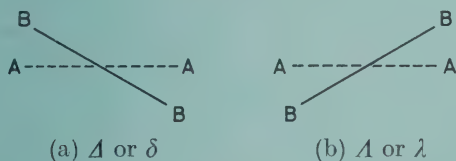


Fig. 3 The figure shows pairs of non-orthogonal skew lines in projection upon a plane parallel to both lines. The fully drawn line BB is above the plane of the paper, the dotted line AA below this plane. (a) corresponds to (a) of Fig. 2 and defines a right-handed helix. (b) corresponds to (b) of Fig. 2 and defines a left-handed helix

* It should be noted that orthogonal to the common normal of the two skew lines there is a two-fold axis (in fact, there are two such axes) of proper rotation which brings each one of the skew lines into coincidence with the other. This means that the helix which the first line, BB , say, determines around the second one, AA , has the same helicity as that which the second one determines around the first one.

** In connection with the singularities mentioned above it should be noted that by moving the ligators away from the ideal octahedral positions a gradual transition from the situation of Fig. 3 (a) to that of Fig. 3 (b) is possible without a change of absolute configuration. However, for this to occur the distortions must be so great that one would no longer think of calling the complex octahedral. Further such cases are unknown.

Two heavy line edges which are neither neighbouring edges having a common vertex, nor opposite edges, will in an octahedron form a pair of skew lines. This pair always has the same relative position as that of a *cis*-bis-bidentate complex.

In Fig. 4 is seen the representation of the *cis*-bis-bidentate complex of Fig. 1 (b) redrawn so as to conform to Fig. 3, and for the particular absolute configuration to Fig. 3 (a). To the corresponding tris complex [Fig. 1 (a)] is attributed the same designation because its three heavy line edges are equivalent and therefore also the three possible pairs of heavy line edges. This is illustrated in Fig. 5.



Fig. 4 The bis-bidentate complex of Fig. 1 (b) redrawn so as to become associated with Fig. 3 (a) and thus to become designated by Δ

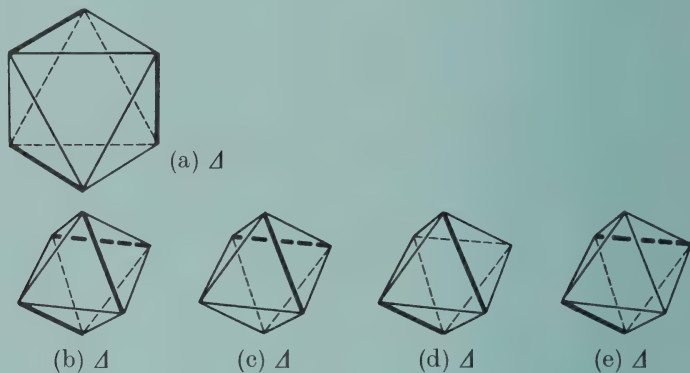


Fig. 5 (a) and (b) show the tris-bidentate system of Fig. 1 (a) redrawn in two different ways. Since each of the bidentate ligands has lost its individuality by being represented only by the edge which it spans, the threefold axis of symmetry of the octahedron applies also to the present system. (a) shows the system in projection on a plane orthogonal to its threefold axis.

(c), (d), and (e) each illustrates one of the three possible pairs of bidentate ligands oriented so as to refer to (b). (c) is associated with Fig. 3 (a), and thus is designated by Δ . The same must hold true also for (d) and (e) because the threefold axis makes the three pairs of representations of bidentate ligands equivalent

3.2 Some examples of polydentate systems

It is straightforward to extend the application of the above rules to more complex situations involving polydentate ligands. It is by analogy with the tris-bidentate case (Fig. 5) only a matter of studying the interrelations between all the chelate rings whose corresponding edges form a pair of skew lines, *i.e.* all the ring pairs whose relative position is the same as in a *cis*-bis-bidentate complex. Now one might count up all such contributions and designate the complex situation by Δ if the number of Δ contributions from

the individual pairs exceeds the number of Δ contributions and vice versa. This convention, which could be applied to the situations shown in Fig. 6–8, will *not* be recommended here for the reason given in the next paragraph. Even though non-helical situations will always contribute Δ and Λ an equal number of times (Fig. 9), the same may be true as well for certain helical situations, as illustrated in Fig. 10.

A case such as that of Fig. 10 requires a further convention and here no simple one has yet been proposed. A possible convention here might conflict with the above simple counting of Δ and Λ contributions. We therefore recommend, at the present stage, for the case of Fig. 6–8 where the number of Δ and Λ contributions is different, to characterize the complexes as follows: Fig. 6, “skew chelate pair, Δ ”; Fig. 7, “skew chelate pair, Λ ”; Fig. 8, “skew chelate pairs, $\Delta\Delta\Lambda$ ”. In the last example the order of the Greek letter symbols is immaterial. The case of Fig. 10 might at present be characterized by (“the end chelate rings form a skew chelate pair, Λ ”).

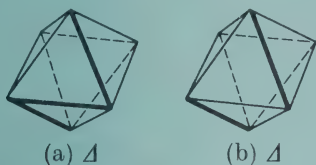


Fig. 6 A quadridentate system (a). Here only two of the heavy line edges are skew, the pair (b) being associated with Fig. 5 (d) and thus being designated by Δ . The system as a whole is proposed designated “skew chelate pair, Δ ”. The system may be thought of as representing the α -isomer of a trien-complex (trien = triethylenetetramine)

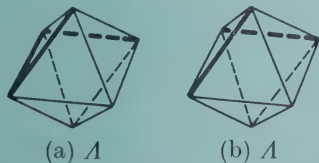


Fig. 7 Another quadridentate complex (a). As in Fig. 6 there is only one helical pair (b). This is clearly associated with the mirror image of Fig. 5 (c) (and, of course, therefore, also of Fig. 5 (d) and (e), although this is less easy to see) and thereby gives rise to the designation Λ . The system is therefore designated “skew chelate pair, Λ ”. The system may represent the β -isomer of a trien-complex (see Fig. 6)

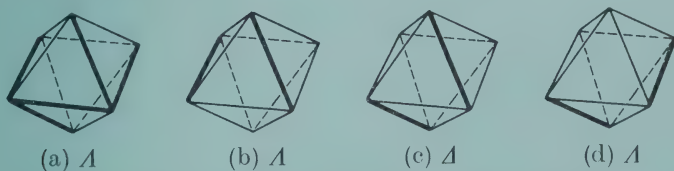


Fig. 8 A sexidentate complex (a). The pair (c) is associated with Fig. 5 (d) and is therefore Δ . The pairs (b) and (d) are clearly the mirror images of Fig. 5 (c) and 5 (e), respectively, and are therefore both Λ . The whole system is designated “skew chelate pairs, $\Delta\Delta\Lambda$ ” where the order of the symbols is immaterial. The system may represent an EDTA complex (EDTA = Ethylenediaminetetraacetic acid)



Fig. 9 A non-helical system (a). The helical pairs (b) and (c) are mirror images of each other and contribute Δ and Λ , respectively. Non-helical systems always have an equal number of Δ and Λ contributions. The reverse conclusion, however, is not valid (see Fig.10)



Fig. 10 A quinquidentate system (a). (b) is Δ by association with Fig.5(c), (c) is Λ because it is the mirror image of (b).

A designation for the whole helical system (a) cannot be obtained without a further convention. A preliminary designation might be "the end chelate rings form a skew chelate pair, Λ "

4. Application to conformation

In order to define the helicity of a ring conformation a convention is required for making a choice of a pair of skew lines. Here it is proposed to choose one of the lines of this pair as the edge covered by the chelate ring, i.e. the line AA joining the two ligators. The other line BB is taken as that joining the two ring atoms which are neighbours to each of the ligators.

Two enantiomeric situations are shown in projection in Fig.11. The two ligators AA are in the plane of the paper, the central atom M is below this plane and the two neighbouring ring atoms BB are above it. Fig.11 (a) and (b) are associated with the corresponding Fig.3, and the proposed convention for designating the helicity is thereby given. In Fig.12 is shown a situation to which is attributed the same designation as that of the case of Fig.11 (a). In Fig.13 BB is parallel to AA and the chelate ring will not be helical at least up to a ring size of seven or eight members, which for our purpose is without importance. The situation in which BB is parallel to AA corresponds to the case of any planar chelate ring, and in addition to this, for a five-membered ring, it corresponds to the envelope form, and for the six-membered ring, either to the chair or to the boat form. In this case only the skew-boat form has a helical character.

Non-helical situations may still represent chiral situations when the chemical significance of the atoms, i.e. their possibility of being different, is considered. The present nomenclature problem, however, is not concerned with such cases.

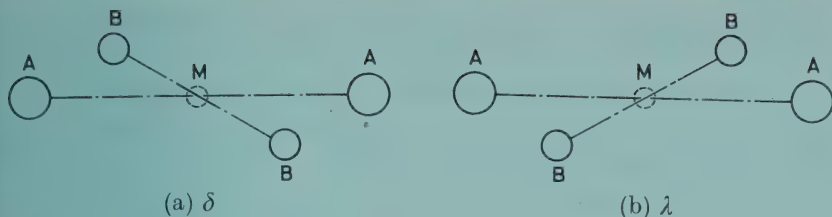


Fig. 11 Illustration of the convention for designating the helical character of the conformation of chelate rings. The ligating atoms in the plane of the paper determine one of our skew lines AA . The neighbouring-atoms of each ligator determine the other line BB , which here is above the plane of the paper, the central atom M being below this plane. The designations become clear by comparison with Fig.3 (a) and (b)

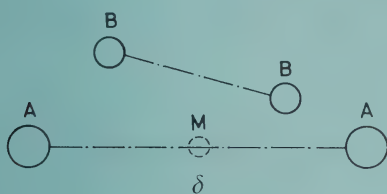


Fig. 12 Illustration of an alternative situation to that of Fig.11 (a). Both atoms BB are above the plane determined by M and AA , but this is immaterial from a nomenclature point of view. The lines AA and BB are still skew and correspond to the situation of Fig.3 (a)



Fig. 13 Non-helical chelate ring drawn as in Fig.11. This figure illustrates a five-membered ring in its envelope form or a six-membered ring in either its boat or its chair form

5. Examples of a few absolute configurations

The proposals which have been put forward here dictate that the absolute configuration of the tris(ethylenediamine)cobalt(III) ion with a positive rotation at the Na_D line be characterized as upper case Λ and (—)propylenediamine in its stable chelate conformer (equatorial CH_3 -) be characterized by lower case λ .

6. Phenomenological characterization

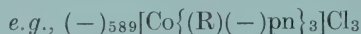
As well as the symbols for designating structure some phenomenological description of a mirror-image isomer is essential. The isomer might be denoted by its sign of rotation at a particular wavelength, $(+)_\lambda$,

e.g., $(+)_589[\text{Co}(\text{en})_3]\text{Cl}_3$ en = ethylenediamine

When optically active ligands are coordinated they are denoted as (+) and (−) where the signs are the signs of rotation of the ligand at the Na_D line,

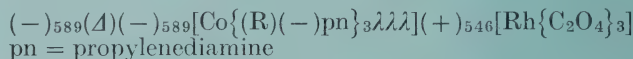
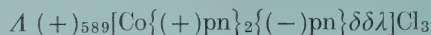


In those instances where the absolute configuration of the ligand is known this might also be included in the description,



7. Full characterization

Examples of the use of the full nomenclature proposed here follow:



8. Rules for the designation of configurational chirality caused by chelation in six-coordinated complexes based on the octahedron

8.1 *Cis-bis-bidentate chelation*

The two ligating atoms of a chelate ring define a line. Two such lines for the pair of chelate rings define a helix. One line is the axis of the helix and the other is the tangent of the helix at the common normal for the skew lines. The tangent describes a right-handed (Δ) or a left-handed (Λ) helix with respect to the axis and thereby defines the configuration.

8.2 *Tris-bidentate chelation*

Any one of the three possible pairs of chelate rings is chosen to designate the configuration by rule 1.

8.3 *Multidentate chelation*

Chiral complexes of multidentate ligands are considered to contain pairs of skew lines (rule 1) and are designated by all the symbols, Δ 's and Λ 's, belonging to all the skew-line pairs. The order of citation of the symbols is immaterial.

9. Rule for the designation of conformational chirality of a chelate ring

The line joining the two ligating atoms and the line joining the two atoms of the chelate ring adjacent to each of the ligating atoms define a helix. One line is the axis of the helix and the other is the tangent of the helix at the common normal for the skew lines. The tangent describes a right-handed (δ) or a left-handed (λ) helix with respect to the axis and thereby defines the conformation.

Appendix

Relationship between the proposed symbols and those in earlier use

The symbols Δ and Λ were originally proposed for tris-bidentate complexes by PIPER¹ who used the threefold axis (C_3) as reference axis. The present convention agrees with the results of PIPER's proposal. The present convention for designation of conformation likewise agrees with LIEHR'S² proposed use of δ and λ .

The absolute configuration³ of $(+)_589[\text{Co}(\text{en})_3]^{3+}$ (in the crystal, $\Delta \delta\delta\delta$) is Δ and that⁴ of $(-)_589[\text{Co}\{(-)\text{pn}\}_3]^{3+}$ is $\Lambda \lambda\lambda\lambda$, as determined by SAITO *et al.* from X-ray crystallography. These two complex ions were in the X-ray papers designated by D and L , respectively. MASON pointed out that the helical configuration about a C_2 axis of a tris-bidentate or *cis*-diacidobis-bidentate complex is opposite to that about the respective C_3 or pseudo C_3 axes. He proposed⁵ the use of P (positive for right-handed) and M (minus for left-handed) as in $P(C_3)$ or $M(C_2)$ where the reference axis is indicated. The result of the present proposal is equivalent to that using the C_3 or pseudo C_3 axis and is *opposite* to that using a C_2 axis, i.e., Δ for $P(C_3)$ or $M(C_2)$ and Λ for $M(C_3)$ or $P(C_2)$. HAWKINS and LARSEN⁶ defined an octant sign to characterize the helicity of configurations (also of polydentate systems) as well as for conformations. For tris-bidentate and *cis*-bis-bidentate systems and for conformations of five and six-membered rings the relation to the present proposal is Δ (positive octant sign), λ (negative octant sign). LEGG and DOUGLAS⁷ suggested the general use of the C_2 axis for reference of helicity and a ring-pairing method for assigning the helicity of complexes containing polydentate ligands. The ring pairs chosen to define the helicity are the same as those proposed here. However, because of the C_2 -reference axis their use of Δ and Λ is opposite to that of the present proposal. It should further be noted that both the octant-sign method and the ring-pairing method of characterizing absolute configurations need extra conventions in certain cases of the type discussed here along with Fig. 10.

COREY and BAILAR⁸ and SARGESON⁹ have discussed the concomitant interplay of conformation and configuration in tris-bidentate diamine complexes. These authors designated the conformation of the five-membered ethylenediamine ring as k and k' , but used k and k' in the opposite sense*. With reference to our Fig. 11 the interrelation of δ , λ and k , k' is

COREY and BAILAR		SARGESON
δ	k'	k
λ	k	k'

Acknowledgment: The Commission wishes to express its appreciation of the valuable help offered by Dr. WERNER FENCHEL, professor of mathematics at the University of Copenhagen, by Sir CHRISTOPHER INGOLD and Dr. R. S. CAHN, and by several chemists working with optically active complexes.

* The cause of the confusion with respect to k and k' is an error in the upper drawing of Fig. 3 of COREY and BAILAR's paper!. The ring conformations of the unstable form, the *ob* form $\Delta \delta\delta\delta$, is correctly given as $k'k'k'$ in the lower drawing of their Fig. 3, but the stable form, the *lel* form $\Lambda \lambda\lambda\lambda$, discussed in the text correctly as kkk , appears in the upper drawing of their Fig. 3 as $\Lambda \delta\delta\delta$

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**INTERNATIONAL UNION OF PURE
AND APPLIED CHEMISTRY
UNION INTERNATIONALE DE CHIMIE
PURE ET APPLIQUÉE**

**INFORMATION BULLETIN
NUMBER 34**

XXVTH CONFERENCE

30 June—8 July 1969

CORTINA (ITALY)

APRIL 1969

SECRETARY GENERAL:

Dr R. Morf, Postbox 165, CH-8058 Zürich-Airport (Switzerland)

Cable address: IUPACAIRPORT

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INTRODUCTION

The main purpose of this "Information Bulletin" No.34 is to draw attention to IUPAC's activities in 1969, activities which will have as their focus two main events:

- (1) The XXVth Conference of the International Union of Pure and Applied Chemistry which will be held in Cortina d'Ampezzo (Italy) from 30 June to 8 July 1969.
Our Italian Hosts will provide us a service which guarantees the efficiency of our deliberations. The detailed programme for the XXVth Conference, which in other words is the General Assembly of IUPAC, appears on p. 4.
- (2) The XXIIInd International Congress of Pure and Applied Chemistry and the XIIth International Conference on Coordination Chemistry, both organized by the *Australian Academy of Science* and the special Organizing Committee, presided over by Dr A.L.G. REES. These two events will be held in Sidney, 20-27 August 1969 (see "Information Bulletin" No.33, p.13).

These two Meetings have been singled out as being the highlights of IUPAC's activities besides a number of other scientific meetings which are given hereafter under "Forthcoming events" and in the calendar.

I extend to you a hearty welcome to Cortina.

Very sincerely yours RUDOLF MORF

XXVTH IUPAC CONFERENCE

CORTINA D'AMPEZZO, ITALY, 30 JUNE—8 JULY 1969

Cortina d'Ampezzo, which the Italian National Adhering Organization has chosen for the location of the XXVth Conference, is situated in the Dolomite mountains.

Accommodation and travel

Full details of hotel accommodation and various travel schemes have already been distributed to National Adhering Organizations, Titular and Associate Members, National Representatives, and Observers. Any queries should be addressed to the IUPAC Secretariat (Bank Court Chambers, 2/3 Pound Way, Cowley Centre, Oxford OX4 3YF, England).

The nearest airports are Venice and Innsbruck. Persons proceeding to Venice will find special coaches available in Roma Square, which will take them directly to their hotels in Cortina d'Ampezzo. Anyone travelling via Innsbruck will need to continue his journey by train to Fortezza, where again coaches will be available to transport him to Cortina d'Ampezzo.

Arrangements can be made through the IUPAC Secretariat for provision of visas and for extended stays in Italy either en route to or from the Conference.

Schedule of meetings

Subject to last-minute changes, the Schedule of Meetings is as shown. Details of meeting rooms will be given to everyone on arrival at his hotel and, in addition, will be displayed on the IUPAC Notice Board in the foyer of each hotel. As far as possible, meetings will take place in the hotels at which persons are staying. The meetings of Council, Bureau and Executive Committee will be held in the Savoia Grand Hotel.

Secretariat

During the Conference the IUPAC Secretariat will be located in the Savoia Grand Hotel (Telephone: CORTINA 3201; telegraphic address: ITALCIT IUPAC CORTINA). It will be open daily from 9.00 and provide typing or photocopying facilities to assist Members and Delegates in their work.

In addition, there will be an hostess, fluent in English, in each hotel where meetings are taking place, to deal with inquiries of a general nature.

Reimbursement

For those Titular Members who have requested reimbursement of travel and subsistence at Cortina d'Ampezzo, this will be made at a Bank situated in the main street close to the Savoia Grand Hotel, between 9.00 and 12.30 and 14.30 and 16.00.

Weather and clothing

Formal dress will not be essential for any of the social functions. However, because several functions will take place out of doors, it is desirable to have available some warm clothing since the night temperature will range from 10 to 15 °C. The average daily temperature is about 25 °C.

SYMPOSIUM ON THE CHEMICAL ASPECTS OF AIR POLLUTION

Cortina d'Ampezzo (Italy), 9-10 July 1969

Under the patronage of IUPAC

Part 1: Physical and chemical transformation of pollutants in the atmosphere.

Part 2: Development of methods for the measurement of air pollutants.

Approximative number of participants: 200.

Number of papers expected: 15 short communications.

Invited lecturers (4 plenary lectures): Prof. R. TRUHAUT (University of Paris); Prof. A. LIBERTI (University of Rome); Dr S.R. CRAXFORD (Warren Spring Laboratory); Dr STEWART (Department of Health and Welfare, USA), or Prof. GEORGII (University of Frankfurt).

Summaries of the papers will be distributed to delegates at the Symposium and the final report will be published in: "Pure and Applied Chemistry."

TIME SCHEDULE OF MEETINGS

Meeting of	Monday 30 June	Tuesday 1 July	Wednesday 2 July	Thursday 3 July	Friday 4 July	Saturday 5 July	Sunday 6 July	Monday 7 July	Tuesday 8 July
Council						9-12.30 14-18		9-12.30 14-18	
Bureau					9-12 14-18				9-12 14-18
Division Presidents Executive Committee				9-12 14-18			9-12		
Interdivisional Committee on Nomenclature and Symbols					16-18				
Coordinating Committee for Analytical Methods							14-18		
Finance Committee			9-12						
Standing Committee on Congress Organization and Programmes			16-18						
Industrial Members of IUPAC					19-21				
Physical Chemistry Division									
Division Committee		9-12							
Commission I.1								9-12	
Physico-Chemical Symbols, Terminology and Units	9-30-12 14-18	9-30-12 14-18	9-30-12 14-18						
Commission I.2				9-12 14-18	9-12				
Thermodynamics and Thermochemistry			14-18	14-18					
Commission I.3			9-12	9-12	9-12				
Electrochemistry				14-18					
Commission I.4			9-12	9-12					
Data and Standards		14-18	14-18						
Commission I.5									
Molecular Structure and Spectroscopy				9-12 14-18					

Meeting of	Monday 30 June	Tuesday 1 July	Wednesday 2 July	Thursday 3 July	Friday 4 July	Saturday 5 July	Sunday 6 July	Monday 7 July	Tuesday 8 July
Commission I.6 Colloid and Surface Chemistry Joint Meeting of Chairmen and Secretaries of I.3 and V.5			9-12 14-18 14-18	9-12 14-18 	9-12 14-18				
Inorganic Chemistry Division									
Division Committee				14-18	18-20				
Commission II.1			9-12	9-12					
Atomic Weights									
Commission II.2	9-12	9-12	9-12	9-12	9-12				
Nomenclature of Inorganic Chemistry	14-18	14-18	14-18	14-18	14-18				
Commission II.3					9-12				
High Temperatures and Refractories									
Organic Chemistry Division									
Division Committee							14-18		
Commission III.2			9-12	9-12					
Chemical Plant Taxonomy			14-18						
Macromolecular Division									
Division Committee		10.30-12 14-19	17-20						
Analytical Chemistry Division									
Division Committee									
Commission V.1		9-12	9-12	14-18					
Analytical Reactions and Reagents									

Meeting of	Monday 30 June	Tuesday 1 July	Wednesday 2 July	Thursday 3 July	Friday 4 July	Saturday 5 July	Sunday 6 July	Monday 7 July	Tuesday 8 July
Commission V.2									
Microchemical Techniques and Trace Analysis		9-12 14-18	9-12 14-18						
Commission V.3					9-12				
Analytical Nomenclature		14-18	14-18						
Commission V.4									
Spectrochemical and other Optical Procedures for Analyses	16-18	9-12 14-18	9-12 14-18						
Commission V.5		9-12	9-12		9-12				
Electroanalytical Chemistry		14-18							
Commission V.6			9-12						
Equilibrium Data			14-18						
Commission V.7									
Analytical Radiochemistry and Nuclear Materials		9-12 14-18	9-12 14-18						
Liaison Meeting on Separation Processes (V.3, V.6)		9-12							
Joint Meeting of V.1 and VI.1.2		14-18							
Joint Meeting of Chairmen and Secretaries of I.3 and V.5									
Open Meeting of Analytical Chemistry Division			14-18	9-12	14-18				
Applied Chemistry Division									
Division Committee	14-18								
Section VI.1			9-12	18-20 9-12					
Food					14-16				
Commission VI.1.1			10-12	9-12	9-12				
Trace Substances			14-18						
Commission VI.1.2			10-12	9-12	9-12				
Food Additives			14-18						
Section VI.2		9-12	9-12						
Permentation Industries		14-18	14-18						

Meeting of	Monday 30 June	Tuesday 1 July	Wednesday 2 July	Thursday 3 July	Friday 4 July	Saturday 5 July	Sunday 6 July	Monday 7 July	Tuesday 8 July
Section VI.3 Oils and Fats			9-12 14-18						
Section VI.4 Toxicology and Industrial Hygiene		9-12 14-18	9-12						
Section VI.5 Pesticides		9-12					9-12		
Commission VI.5.1 Terminal Pesticide Residues		14-18	9-12 14-18	9-12	9-12 14-18	14-18 9-12			
Commission VI.5.2 Pesticide Residue Analysis									
Section VI.6 Organic Coatings		9-12 14-18	9-12 14-18 9-12						
Section VI.8 Water, Sewage and Industrial Wastes			14-18						
Joint Meeting of V.1 and VI.1.2		14-18		14-18					
Open Meeting of Applied Chemistry Division				14-18					

Social Functions

A full social programme has been arranged by our hosts in Cortina for all IUPAC Members, National Delegates and their families as follows:

Ice-hockey Match at the Olympic Stadium	Wednesday, 2 July
Reception by Aziende Autonome Soggiorno e Turismo	Thursday, 3 July
Reception by the Municipality of Cortina d'Ampezzo	Saturday, 5 July
Reception by the Italian Research Council	Sunday, 6 July

In addition there will be a full day and a half-day excursion in the Dolomites for wives of Members and Delegates to the Conference.

DETAILED INFORMATION REGARDING FORTHCOMING EVENTS

SECOND INTERNATIONAL PRE-SYMPOSIUM ON CAROTENOIDS OTHER THAN VITAMIN A

6-9 May 1969, New Mexico State University, Las Cruces (New Mexico)

*Sponsored by the International Union of Pure and Applied Chemistry
(Organic Chemistry Division), Hoffmann-La Roche, Inc., Nutley, New
Jersey, and New Mexico State University*

The First International Pre-Symposium on Carotenoids was at the Norwegian Institute of Technology, Trondheim, June 1966, with the sponsorship of IUPAC. Plans have been made to have a similar symposium this spring and the program is very nearly completed.

The program will include four main lectures, a series of session lectures related to topics of the main lectures and contributed research papers. Topics for main lectures are physical organic studies of carotenoids, structure of natural carotenoids and biosynthesis. The principal lecturers will be Dr U. SCHWIETER, Dr S. L. JENSEN, Dr JOHN W. PORTER and Prof. T. W. GOODWIN. Session lectures will include the topics: X-ray crystallography, ORD, mass spectrometry, cyclization reactions, total synthesis, and biosynthesis and function. Research papers may be contributed but will be restricted to studies of carotenoids.

Forms for registration, the program and the request for contributed research papers will soon be mailed.

Further inquiry may be sent to:

Prof. O. B. WEEKS, Research Center, New Mexico State University, Las Cruces, New Mexico 88001

THE CHEMICAL INSTITUTE OF CANADA

Ottawa 4, Ontario (Canada)

The Chemical Institute of Canada, 151 Slater Street, Ottawa 4, Ontario, has scheduled the following meetings for 1969 and 1970:

25-28 May 1969

52nd Canadian Chemical Conference and Exhibition, Queen Elizabeth Hotel, Montreal, Que. Contact CIC, 151 Slater Street, Ottawa 4, Ont.

17-24 August 1969

3rd NMR Symposium, cosponsored by Physical Chemistry Division and University of Toronto, Toronto, Ont. Contact CIC, 151 Slater Street, Ottawa 4, Ont.

27–29 August 1969

Symposium on Multiple Bonding in Inorganic Chemistry, University of Manitoba, Winnipeg, Man. Sponsored by Inorganic Chemistry Division, CIC. Contact Dr W.A. G. GRAHAM, Department of Chemistry, University of Alberta, Edmonton, Alta.

3–5 September 1969

15th Canadian High Polymer Forum, Queen's University, Kingston, Ont. Sponsored by CIC Macromolecular Science Division. Contact Dr R. ST. JOHN MANLEY, Pulp and Paper Research Institute, 570 St. Johns Road, Pointe Claire, Que.

19–22 October 1969

19th Canadian Chemical Engineering Conference, The Canadian Society for Chemical Engineering, incorporating the 3rd Symposium on Catalysis, sponsored by the Physical Chemistry Division, CIC. Contact Dr D.B. ROBINSON, Department of Chemical and Petroleum Engineering, University of Alberta, Edmonton, Alta.

25–29 May 1970

Joint National Meeting, The Chemical Institute of Canada and the American Chemical Society, Toronto, Ont. Contact CIC, 151 Slater Street, Ottawa 4, Ont.

5TH RUDOLFS RESEARCH CONFERENCE

Rutgers, N.J. (USA), 30 June–2 July 1969

The 5th Rudolfs Research Conference will be held at Rutgers, The State University, New Brunswick, New Jersey, on 30 June, 1 and 2 July 1969. The theme of this conference will be: "Origin, distribution, transport, and fate of organic compounds in aquatic environments." Further details may be obtained from Mr ROGER LOCANDRO, Office of Resident Instruction, Room 206, College of Agriculture and Environmental Sciences, Rutgers, The State University, New Brunswick, N.J. 08903.

INTERNATIONAL ATOMIC ABSORPTION SPECTROSCOPY CONFERENCE

Sheffield, 14–18 July 1969

An International Atomic Absorption Spectroscopy Conference, organized by the Atomic Absorption Spectroscopy Group of the Society for Analytical Chemistry in association with the Spectroscopy Group of the Institute of Physics, is being held in Sheffield from 14–18 July 1969. This Conference, which is sponsored by IUPAC, is intended to cover all aspects of atomic absorption and atomic fluorescence spectroscopy, and closely related techniques. Many internationally known workers will be attending, several of whom will be presenting plenary lectures at the start of each session. The programme, consisting of plenary lectures and contributed papers will include sessions on the following topics:

- Theoretical aspects of atomic absorption and allied phenomena
- Atomic fluorescence spectroscopy

- Fundamental developments in instrumentation
- New developments in the analytical use of flames
- New techniques in the analysis of biological, metallurgical and ceramic materials
- General analytical development

Contributed papers are cordially invited for the Conference. The last date for receipt of extended abstracts (approx. 700 words) is 28 February 1969.

INTERNATIONAL SYMPOSIUM ON THE CHEMICAL CONTROL OF THE HUMAN ENVIRONMENT

Johannesburg (South Africa), 14-18 July 1969

The Bureau of the International Union of Pure and Applied Chemistry (IUPAC) has agreed to sponsor a symposium on "The Chemical Control of the Human Environment" to be held at the University of the Witwatersrand, Johannesburg (South Africa), from 14-18 July 1969. The symposium is being organized jointly by the South African Chemical Institute and the South African Council for Scientific and Industrial Research.

The theme of the symposium will be chemistry in relation to environmental control.

Papers

The Scientific Programme Committee will consider any papers of special interest dealing with chemical topics relating to the control of the environment. This includes all chemical and biochemical problems arising from the use of chemicals for control of the human environment and also the isolation, analysis and identification of injurious chemical substances. The symposium will be divided into five separate sections, each of which will be introduced by at least one plenary lecture given by a leading scientist in a particular field.

Sections

The five sections are subdivided as follows:

- *The control of air pollution:* (a) Measurements of pollution, (b) chemical and chemical engineering control of emission, (c) chemical reactions in the atmosphere.
- *The control of water supplies:* (a) Control of municipal and industrial effluents, (b) treatment of water supplies, (c) reuse of effluents.
- *The control of agricultural pests:* (a) Insect control, (b) control of virus and fungus diseases, (c) use of herbicides, (d) control of residues.
- *The control of health:* (a) Chemical additives in animal nutrition and health, (b) chemical control of the vectors of bilharzia and malaria, (c) control of residues from pesticides and from radioactive fallout, (d) control of food additives.
- *The control of toxic substances of biological origin:* (a) Chemistry and analysis of mycotoxins, (b) biochemistry of mycotoxins, (c) chemistry of other microbial toxins, (d) chemistry of plant toxins.

Plenary lectures

The following distinguished overseas scientists have been invited to deliver the plenary lectures:

Prof. Dr. WOLFGANG TESKE (Germany): "Control of air pollution"

Prof. K.J. IVES (USA): "Control of water supplies"

Prof. F. A. GUNTHER (USA): "Control of agricultural pests"
Prof. A. S. CRAFTS (USA): "Control of agricultural pests"
Dr L. A. GOLDBLATT (USA): "Control of toxic substances"
Prof. R. TRUHAUT (France): "Control of toxic substances"
Prof. L. GOLBERG (USA): "Control of health"
Prof. W. HUBER (USA): "Control of health"

Abstracts. Intending contributors of papers are asked to complete the attached application form which must reach the Symposium Secretary, together with the title and abstract of their proposed paper in English. Abstracts should not exceed 300 typewritten words.

As it is anticipated that the number of papers offered will exceed the number that can be conveniently and efficiently presented, the Organizing Committee retains the privilege of reviewing and selecting the papers that will appear in the final programme.

Presentation of papers. The presentation of papers at the Symposium will be limited to 20 minutes, which includes the time for the projection of slides (mounted 35 mm) or showing of illustrations by means of an overhead projector, followed by a 10-minute period for discussions.

A book of abstracts of all papers accepted for the Symposium will be issued to delegates on registration at the Symposium.

Symposium language. While the plenary lectures will be given in English, contributed papers may be presented in any language. The organizers suggest, however, that speakers should use a language commonly understood by most delegates, as no arrangements can be made for simultaneous translation. All Symposium literature will be published in English.

Technical excursions and social events. A full range of technical excursions and social events has been included in the Symposium programme. These excursions will include visits to the South African Council for Scientific and Industrial Research in Pretoria, the Veterinary Research Institute of the Department of Agricultural Technical Services at Onderstepoort, and African Explosives and Chemical Industries Ltd. Social functions will include a cocktail party and a banquet as well as a South African "braaivleis".

The registration fee covers the cost of teas, luncheons as well as participation in all technical excursions and social functions, with the exception of the banquet, for which an additional fee of R5.00 per head will be charged.

Ladies' programme. A programme specially designed to be of interest to the ladies, has been planned and will include sightseeing tours of Johannesburg and Pretoria. A registration fee of R4.00 per head covers the cost of participation in the above programme and includes teas, luncheons, etc.

Post-Symposium tours. A programme of post-Symposium tours designed to suit delegates wishing to stay after the Symposium, can be arranged and details relating to recommended tours giving costs and dates are enclosed.

Accommodation. Hotel accommodation can be reserved for the period of the Symposium and accommodation will also be available in modern University residences.

Please note that only limited double accommodation will be available at University residences.

The current hotel tariffs for bed and breakfast per day, with private bath are:

	Double	Single
Sunnyside Park Hotel	R15.00	R8.00
Cranbrooke Hotel	10.00	5.50
University residences	2.50 per person per day	

Transportation. Buses will transport delegates daily to and from the abovementioned hotels and University residences to the University of the Witwatersrand.

Registration fee. R15.00 per person (R1.720 = £1 sterling and R0.718 = US\$1 at current exchange rates). Delegates from foreign countries are requested to pay their fees in South African currency by bank draft. Other delegates may pay by cheque or money order which must be crossed and made payable to IUPAC Symposium – CSIR. Registration fees must be paid before 30 May 1969.

Information: IUPAC Symposium Secretary, c/o SA Council for Scientific and Industrial Research, PO Box 395, Pretoria (Republic of South Africa).

VIIITH INTERNATIONAL CONGRESS OF NUTRITION

Prague, 28 August–5 September 1969

The International Union of Nutritional Sciences invites to the VIIIth International Congress of Nutrition at Prague, organized in the Technical University of Prague.

1969 PRAGUE MICROSYMPOSIA ON MACROMOLECULES

Prague, 1–11 September 1969

The Institute of Macromolecular Chemistry of the Czechoslovak Academy of Sciences and the Scientific and Organizing Committee have the pleasure of inviting you to participate in the 1969 Prague meetings, sponsored by IUPAC:

- Rheology of polymer solids and concentrated solutions, 1–4 September 1969
- Cyclopolymers and cyclopolymerization, 1–3 September 1969
- Light scattering in polymer science, 8–11 September 1969.

INTERNATIONAL SYMPOSIUM ON UNIVERSITY CHEMICAL EDUCATION

Frascati (Rome), 16–19 October 1969

An International Symposium on University Chemical Education will be held at Frascati (Rome), sponsored jointly by the National Council of Research of Italy (CNR, Rome) and the IUPAC Committee on the Teaching of Chemistry. The Organizing Committee is Prof. G. GIACOMETTI, G. ILLUMINATI, R. S. NYHOLM, R. W. PARRY and G. SARTORI. The Symposium will be held under the chairmanship of Prof. Sir RONALD NYHOLM; the general secretary will be Mr DENNIS G. CHISMAN, Secretary IUPAC Committee on the Teaching of Chemistry.

The principal topics to be discussed are:

1. *The scope of chemical education*
 - Nature and duration of degree courses in chemistry
 - Teaching organization: traditional (i.e. organic, inorganic, physical, etc.) versus alternate division (structure, dynamics, mechanisms, etc.)
 - Contents, teaching methods, teaching aids
 - Practical courses
 - Student assessments and examinations
 - Teaching of mathematics and physics
2. *Research training (postgraduate)*
3. *Departmental organization and industrial contacts*
 - Organization with respect to teaching and research
 - Staff responsibilities and government
 - Relations with industry: what industry expects from the university, what the university expects from industry.

The Symposium will be restricted in numbers and most of the participants will be specially invited. A circular giving further details may be obtained from Prof. G. ILLUMINATI, Istituto chimico, Università di Roma, 00185 Roma (Italy).

7TH INTERNATIONAL SYMPOSIUM ON THE CHEMISTRY OF NATURAL PRODUCTS

Riga, 22-27 June 1970

The meeting will take place in the buildings of the Latvian Academy of Sciences, Riga, USSR, during the period 22-27 June 1970.

Scientific programme

The Symposium will be devoted mainly to the chemistry of biologically active biopolymers and bioregulators. Within the meeting it is proposed to organize separate sections on the following topics:

- | | |
|---|---|
| A | Peptides and proteins |
| B | Nucleotides and nucleic acids |
| C | Lipids (including physical chemistry of membranes) |
| D | Carbohydrates |
| E | Other natural products (steroids, terpenoids, alkaloids, antibiotics, etc.) |
| F | Physical methods |

Symposium lectures

There will be twelve main Symposium lectures to be given by the following distinguished scientists:

Prof. D. H. R. BARTON (UK), Prof. L. L. M. VAN DEENEN (Netherlands), Prof. C. DJERASSI (USA), Prof. H. G. KHORANA (USA), Prof. D. E. KOSHLAND (USA), Prof. E. LEDERER (France), Prof. K. NAKANISHI (Japan), Prof. V. PRELOG (Switzerland), Prof. M. M. SHEMYAKIN (USSR), Prof. F. ŠORM (Czechoslovakia), Prof. F. B. STRAUB (Hungary) and Prof. R. B. WOODWARD (USA).

Contributed papers

The Scientific Programme Committee will consider papers of special interest and novelty in any branch of Natural Product Chemistry. Members wishing to present a paper at the Symposium will have to submit an abstract and to complete the application forms to be distributed with Circular 2. The abstracts and the applications to contribute a paper for the meeting must reach the Secretary not later than 1 February 1970.

Symposium languages

The official languages of the Symposium will be English and Russian. Contributed papers may be presented in any languages, but the organizers suggest that speakers should use a language that is commonly understood by most participants as no arrangements will be made for simultaneous translation. The Symposium literature will be published in English and Russian.

Social events, tours and ladies programme

A full programme of social events is planned including sight-seeing excursions in and about Riga. A ladies programme will also be arranged.

Accommodation

Reservation will be available for the period of the Symposium in hotels and hostels. Detailed information will be given in Circular 2.

Provisional applications and Circular 2

Those planning to attend the Symposium are requested to complete and return the form as soon as possible. This provisional application will imply no obligation but will ensure receipt of Circular 2 which will be distributed in November 1969. Circular 2 will include forms for: registration, submission of contributed papers, participation in main social events, and accommodation.

Executive committee

YU. A. OVCHINNIKOV (Chairman), S. N. ANANCHENKO (General Secretary), V. K. ANTONOV, E. I. BUDOWSKY, G. G. CHAKHMAKHCHEV, G. I. CHIPEN, S. A. GILLER (Vice-Chairman), A. Ya. KHORLIN, A. S. KHOKHLOV (Chairman, Scientific Programme Committee), I. N. KISELEV, M. N. KOLOSOV, S. G. KORNEEV, M. I. ROKHLIN, V. M. STEPANOV, I. I. LOVAROVA and I. V. TORGOV.

Presymposia

Provisional plans have been made to arrange three presymposia of restricted scope with a limited number of participants on the following topics:

- A *Mechanism of enzyme catalysis* (Chairman: Prof. A. E. BRAUNSTEIN)
- B *Physico-chemical basis of transport through biological membranes* (Chairman: Prof. L. D. BERGELSON)
- C *Antibiotics: Chemistry and mode of action* (Chairman: Prof. A. S. KHOKHLOV)

The presymposia will be held in Riga, 19–20 June 1970.

Correspondence

Correspondence related to the meetings should be addressed to: Prof. (Mrs) S.N. ANANCHENKO, General Secretary, 7th International Symposium on the Chemistry of Natural Products, Institute for Chemistry of Natural Products, USSR Academy of Sciences, Ul. Vavilova 32, Moscow 312, USSR. Cables: Moscow 312 Bioorganica.

INTERNATIONAL SYMPOSIUM ON THE CHEMISTRY OF NONBENZENOID AROMATIC COMPOUNDS

Sendai (Japan), 24-28 August 1970

The programme under the chairmanship of Prof. TETSUO NOZOE will include the following topics:

- Carbocyclic nonbenzenoid aromatic compounds
- Novel heteroaromatics
- Metal complexes with aromatic character
- Others

There will be about ten invited lectures by Prof. R.BRESLOW (USA), Prof. M.J.S. DEWAR (USA), Prof. W. E. VON DOERING (USA), Prof. K.HAFNER (Germany), Prof. E. HEILBRONNER (Switzerland), Prof. T.NAKAJIMA (Japan), Prof. H.PRINZBACH (Switzerland), Prof. F.SONDHEIMER (UK), Prof. E.VOGEL (Germany), and Prof. M.E. VOLPIN (USSR).

All correspondence concerning the symposium should be addressed to Prof. SHÔ ITÔ, General Secretary, Department of Chemistry, Tohoku University, Sendai (Japan).

REPORTS ON IUPAC ACTIVITIES

IVth INTERNATIONAL CONGRESS ON CATALYSIS

Moscow, 23-29 June 1968

The 4th International Congress on Catalysis, sponsored by the Academy of Sciences of the USSR, was held in Moscow. The Organizing Committee consisting of 28 members, was headed by the Member of Academy of Sciences of the USSR Prof. B.A. KAZANSKII.

The Congress was devoted to the discussion of the problem of catalytic action prediction, which is in fact one of the most important problems in the theory of catalysis. The discussion of this problem is of the greatest significance, as its solving would contribute to scientific and industrial progress.

The Congress was followed by three Symposia; at the Moscow ones the "Mechanisms and kinetics of complex catalytic reactions" (1-3 July) and "Electronic phenomena in chemisorption and catalysis on semiconductors" (2-4 July) were discussed. The third Symposium took place in Novosibirsk (5-7 July) with the "Porous structure of catalysts and the role of transport processes in heterogeneous catalysis" as the main topic.

Special lectures were delivered at the Congress:

- "Mobility on pore systems especially with respect to the selectivity problems", by Prof. J.H. DE BOER (Netherlands)
- "The significance of electronic factors and of internal cybernetics of the processes in the prediction of catalytic properties", by Prof. S.Z. ROGINSKII (USSR)
- "Crystal and ligand field models of solid catalysts", by Prof. D.A. DOWDEN (UK)
- "The structure and stability of hydrocarbon intermediates on the surface of catalysts", by Prof. C. KEMBALL (UK)
- "Catalysis by metals", by Prof. G. RIENÄCKER (GDR); because of Prof. RIENÄCKER's illness this lecture was read by Dr VÖLTER
- "Linear free energy relationships in heterogeneous catalysis. Thermodynamic and quantum-chemical approaches", by Prof. Y. YONEDA (Japan).

The following lectures were delivered at the Symposium "Mechanism and kinetics of complex catalytic reactions":

- "The mechanism and kinetics of some reactions on silica-alumina catalysts", by Prof. J.H. DE BOER (Netherlands)
- "Some problems of homogeneous catalysis", by Prof. N.N. SEMENOV and Prof. A.E. SHILOV (USSR)
- "Radioisotopes and chromatography in the investigation of complex catalytic reactions", by Prof. G.V. ISAGULIANZ and Dr M.I. YANOVSKII (USSR)
- "Catalytic oxidation of unsaturated hydrocarbons", by Prof. W.M.H. SACHTLER (Netherlands)
- "Kinetics of stationary complex reactions", by Prof. M.I. TEMKIN (USSR)
- "Some aspects of the mechanism of catalytic reactions of hydrocarbons", by Prof. J.E. GERMAIN (France)
- "A statistical interpretation of stereoregular polymerization", by Prof. J. FURUKAWA (Japan)
- "Stereospecific catalytic polymerization of dienes influenced by π -allylic complexes of transition metals", by Prof. B.A. DOLGOPLOSK (USSR). Prof. B.A. KAZANSKII

II^e SYMPOSIUM INTERNATIONAL SUR LA CHIMIE DES COMPOSÉS ORGANIQUES DU SILICIUM

Bordeaux-Talence (France), 9-12 juillet 1968

Le II^e Symposium international sur la Chimie des Composés organiques du Silicium qui s'est tenu à la Faculté des Sciences de Bordeaux à Talence (France) a été organisé par le Laboratoire de Chimie organique de la Faculté des Sciences de Bordeaux. La réunion était placée sous les auspices de l'Union Internationale de Chimie Pure et Appliquée, le Prof. H. NORMANT, membre de l'Académie des Sciences, en assurait la présidence d'honneur, les Prof. R. CALAS et J. VALADE étaient respectivement président et secrétaire général du Comité d'Organisation.

Le programme scientifique comprenait 13 conférences plénières, dont le texte paraîtra dans *Pure and Applied Chemistry*, et 92 communications réparties en 3 séances parallèles.

Les conférences plénières suivantes furent prononcées:

- Prof. R. WEST (USA): «Anionic rearrangements of organosilicon compounds»
- Prof. K. A. ANDRIANOV (URSS): «The polymerization of organosilicon cyclic compounds»
- Prof. U. WANNAGAT (RFA): «Dérivés silicium-azote N-métallés: préparation, structure et réactions»
- Dr D. R. WEYENBERG (USA): «Divalent silicon intermediates in the pyrolysis of alkoxy-polysilanes»
- Prof. G. A. RAZUVAEV (URSS): «Les composés bimétallorganiques du silicium et du germanium»
- Prof. C. EABORN (UK): «Some recent studies of cleavages of silicon-carbon and related bonds»
- Prof. R. A. BENKESER (USA): «The chemistry of trichlorosilane in the presence of tertiary amines»
- Prof. M. G. VORONKOV (URSS): «Physiologically active organosilicon compounds»
- Prof. H. KRIEGSMANN (RDA): «Intra- und intermolekulare Wechselwirkungen in einigen Organo-Silizium-Verbindungen»
- Prof. A. G. MACDIARMID: «Properties of silicon derivatives of cobalt, manganese and iron carbonyls»
- Prof. H. GILMAN (USA): «Silylations of some polyhalogenated compounds»
- Prof. V. BAZANT (Tchécoslovaquie): «To the mechanisms of the reaction of organic halides with silicon»
- Prof. E. FRAINNET (France): «Données récentes sur la réactivité de dérivés organosiliciés notamment d'organosilanes renfermant la liaison SiH»

Le Prof. L. H. SOMMER empêché ne put présenter sa conférence: «Mechanistic pathways of the Si-H bond stereochemical studies». Elle paraîtra cependant dans le volume des textes des conférences.

Le volume des conférences sera publié par Butterworths, London, en 1969. Les résumés des communications ont fait l'objet d'une publication réalisée par le Comité d'Organisation et remise à tous les participants.

Les conférences et communications ont porté sur tous les aspects fondamentaux et d'application de la Chimie des composés organiques du silicium. Elles ont permis de faire le point des derniers développements de ce domaine de la chimie.

Les échanges entre les participants au cours des séances et pendant les différentes manifestations organisées à l'occasion du Symposium, furent nombreux et fructueux.

Le Comité d'Organisation des Symposium sur la Chimie des composés organiques du silicium a décidé de tenir sa prochaine manifestation (III^e Symposium sur la Chimie des composés organiques du silicium) à Madison (USA) en 1972. Le Prof. R. WEST a bien voulu accepter d'organiser cette manifestation.

J. VALADE

VITH INTERNATIONAL SYMPOSIUM FOR THE REACTIVITY OF SOLIDS

New York, 25-30 August 1968

The VIth International Symposium for the Reactivity of Solids was held at the General Electric Research and Development Center in Schenectady, New York, USA. The meeting was organized under the auspices of IUPAC, by sponsors from the Air Force Office of Scientific Research, and the General Electric Company. Prof. J. W. MITCHELL acted as Chairman of the Scientific Committee; Drs P. CANNON, R. W. ROBERTS, and R. C. DEVRIES acted as Secretary, Executive Manager, and Local Chairman, respectively. The scientific program included five plenary lectures, the text of which will be published, along with the contributed papers, by John Wiley and Sons early in 1969. Plenary session speakers were:

Session 1: Dr A. D. WADSLEY, Division of Mineral Chemistry DCIRO, Melbourne (Australia): "Crystallographic shear and planar faults in solids".

Session 2: Dr M. KAHLWEIT, Max-Planck-Institut für Physikalische Chemie, Göttingen (Germany): "On the kinetics of precipitation".

Session 3: Prof. P. W. M. JACOBS, The University of Western Ontario, London, Ontario (Canada): "Thermal and photochemical decomposition reactions in inorganic and organic solids".

Session 4: Prof. KARL HAUFFE, Universität Göttingen, Göttingen (Germany): "Corrosion of metals in gases and aqueous solutions".

Session 5: Dr MORTON E. JONES, Texas Instruments, Inc. Dallas, Texas (USA): "The epitaxial growth of semiconductors".

Session 6: Dr H. SCHMALZREID, Institute for Theoretical Metallurgy, Technische Hochschule Clausthal (Germany): "Chemical reactions between crystalline solids".

Session 7: Dr W. B. HILLIG, General Electric Research and Development Center, Schenectady, N.Y. (USA): "Glass as a medium for controlling physiochemical reactions".

Session 8: Dr C. J. M. ROOYMANS, Philips Research Laboratories, Eindhoven (Netherlands): "Chemical processes in high-pressure systems".

Approximately 180 participants from two dozen countries attended the lectures, as well as the discussions. The main topics concerned the state of knowledge and key problems in the study of solid state chemical reactions, and since the meeting had been organized to maximize discussion, care was taken to explore the limits of current knowledge in a forward-looking way. The sessions were well attended and vigorous discussions ensued.

Besides the scientific program, a welcoming party was held at Union College, Schenectady, on the evening of Sunday, 25 August, and an excursion to Lake George,

New York, was held on Wednesday afternoon, 28 August. The conference banquet was held at the new State University of New York at Albany on Thursday, 29 August; principal guests attending were Dr A.M.BUECHE, Vice-President, General Electric Company, J.ANDERSON, Deputy Director, New York State Atomic and Space Development Authority.

At a business meeting, the Symposium created a standing committee charged with the implementation of the VIIth International Symposium for the Reactivity of Solids, and correspondence concerning the timing and location and content of such a meeting should be directed to PAUL HAGENMULLER, University of Bordeaux, France. Those who wish to obtain copies of the proceedings of the 1968 Symposium are requested to write to John Wiley & Sons rather than to the organizers of that meeting.

2ND INTERNATIONAL SYMPOSIUM "PHARMACEUTICAL CHEMISTRY"

Münster/Westfalen, 22-26 July 1968

The 2nd IUPAC Symposium "Pharmaceutical Chemistry" took place at the University of Münster (Germany). It was organized by Prof. Dr K.E.SCHULTE, Institute for Pharmaceutical Chemistry, University of Münster, under the sponsorship of IUPAC.

The program consisted of the discussion of five topics for which the following plenary lectures served as introductions:

1. Nonsteroid anti-inflammatory drugs

M.W.WHITEHOUSE, Ohio (USA): "Molecular pharmacology of some anti-inflammatory drugs"

K.J.DOEBEL, Ardsley (USA): "The chemistry of nonsteroidal anti-inflammatory agents"

2. Analgetically acting drugs

CH.A.WINTER, Philadelphia (USA): "Analgetic properties of compounds as related to pharmacological action"

G.DE STEVENS, Summit (USA): "The chemistry of some new analgetics"

3. Drugs influencing circulatory system and heart functions

O.KRAUPP, Wien (Austria): "Pharmakodynamische Beeinflussung des Kreislaufes und der Herzfunktion"

M.PROTIVA, Prag (ČSSR): "Entwicklung von neuen Strukturen im Gebiet der Arzneistoffe, die Kreislauf und Herzfunktion beeinflussen"

4. Chemotherapy of parasitic infections

G.N.PERSCHIN, Moscow (USSR): "Die Chemotherapie einiger protozoischer Infektionen (Leishmaniosen, Trichomonosen, Lambliosen und Toxoplasmosen)"

A.BROSSI, Nutley (USA): "Chemical considerations in the experimental approach to the therapy of parasitic infections"

5. *Metabolism of drugs*

E.J. ARIENS, Nijmegen (Netherlands): "Molekularbiologische Grundlagen der Arzneistoffwirkung"

J.J. BURNS, Nutley (USA): "Therapeutic implications of drug metabolism"

A. BECKETT, London (UK): "The importance of steric, stereochemical and physico-organic features in drug metabolism and drug action"

The following main lectures were given in addition:

S. GARATTINI, Milano (Italy): "The open field of pharmacology"

H. TUCHMANN-DUPLESSIS, Paris (France): "Problèmes posés par les retentissements possibles des médicaments sur la progéniture"

E. JUCKER, Basel (Switzerland): "Rechtsschutz auf dem Gebiet der Arzneistoffe"

These lectures will be published in "Pure and Applied Chemistry". 75 original papers concerning topics 1-5 have been delivered.

THIRD INTERNATIONAL FERMENTATION SYMPOSIUM

New Brunswick, N.J. (USA), 2-6 September 1968

The Third International Fermentation Symposium was held on the campus of Rutgers, The State University, New Brunswick, New Jersey. The Symposium was sponsored and organized by the Microbial Chemistry and Technology Division of the American Chemical Society with the Fermentation Industries Section of the Applied Chemistry Division of the International Union of Pure and Applied Chemistry as co-sponsor. The Institute of Microbiology of Rutgers University was host. Financial support of the Symposium was provided by the National Institute of Allergy and Infectious Diseases, Washington, DC, the Foundation for Microbiology as well as 44 industrial concerns.

Attendance at the Symposium was excellent, exceeding that of both preceding Symposia. Seven hundred and thirty-seven scientists and engineers from 27 countries and 5 continents were registered.

The scientific program was built around the theme, "Fermentation advances in the light of recent theoretical progress in microbiology, biochemistry and engineering". The opening ceremonies were followed by two Plenary Lectures on the topic, "Growth and regulation as a basis for obtaining microbial metabolites". Prof. A.B. PARDEE of Princeton University discussed: "Enzyme production by bacteria", while Prof. G.N. COHEN of the National Center for Scientific Research (France) spoke on "Regulation of enzyme activity in microorganisms".

The closing ceremonies also included two Plenary Lectures, one titled: "Ferment or perish: Future role of applied microbiology in world affairs" and the other: "Fermentation in the years ahead" presented respectively by Prof. C.G. HEDEN of Karolinska Institute (Sweden) and Dr A.F. LANGLYKKE of Rutgers University.

During the week, 40 invited speakers from 10 countries presented papers in eight Focal Topic Sessions covering fermentation topics relating to the culture, metabolite biosynthesis, isolation and purification, dynamic phenomena, novel approaches to equipment and design, continuous cultivation, novel microbial products and novel energy sources.

**INTERNATIONAL SYMPOSIUM
ON MACROMOLECULAR CHEMISTRY**

Toronto, Ontario (Canada), 3-6 September 1968

The first major meeting of the new Division of Macromolecular Science of IUPAC was well attended and, in keeping with its predecessors, the major meeting place of polymer scientists from all countries. Some 850 representatives from 25 countries attended the sessions. Canadian hosts were the Canadian High Polymer Forum which is co-sponsored in turn by the National Research Council of Canada and the Division of Macromolecular Science of the Chemical Institute of Canada.

Dr J. E. GUILLET, Symposium Chairman, greeted the delegates and promised them an enjoyable conference with a minimum of formality. The four days which followed were packed with technical sessions, nearly 300 papers in seventeen sessions.

The opening plenary lecture was delivered by Dr H. F. MARK on the subject: "Synthetic polymers in medical science." There were four additional plenary lecturers, one each morning: Prof. KIRSCHNER on "Kinetics of conformational changes in polymers", Prof. KARGIN on "The structure of polymers in the amorphous state", Prof. PHILLIPS on "Three-dimensional structures of globular proteins" and Prof. FLORY on "Configuration and properties of random polymer chains".

There were thirteen sessions on the physical properties and structure of synthetic high polymers each introduced by two invited lecturers who covered some aspect of the state of the science. Topics included thermodynamics in solution, conformation of molecules in solution, polyelectrolytes and their solutions, elucidation of molecular structure such as tacticity and order, electrical properties such as conduction and relaxation processes, plastic deformation and structure in crystalline polymers, adsorption of polymers, rheology of polymer composites blends and suspensions, interfacial phenomena and failure mechanisms of reinforced polymers, network topology and viscoelasticity of elastomers, structure and properties of cellulose, hemicelluloses and lignins, state and transitions in organic and inorganic glasses, and general papers.

A particularly large and active session on biopolymers was also held with four sessions devoted to protein-ligand interactions, structure of biopolymers, nucleic acids, and immunoglobulins. Those in attendance expressed a strong desire to have biopolymers as a regular feature of the International Symposium. Again each session was opened by two invited lecturers.

With all technical sessions in the Royal York Hotel it was easy to move from session to session and to meet individuals for discussions. Social events included scenic and cultural tours for the ladies, tours of the Sheridan Park Research Community, a reception at Casa Loma, a banquet at the Inn-on-the-Park, and a theatre dinner party at Ed's Warehouse (famous for its beef dinners) and the Royal Alexandra Theatre. Delegates who tired of the conference found many attractions in the large diversity of activities in the Metropolitan Toronto area, an extremely cosmopolitan and rapidly expanding megalopolis.

H. L. WILLIAMS

**2ND PRAGUE MICROSYMPOSIUM:
STRUCTURE OF ORGANIC SOLIDS**

Prague, 16–20 September 1968

The 2nd Microsymposium on Structure of Organic Solids took place in Prague (Czechoslovakia). It was organized by the Institute of Macromolecular Chemistry of Czechoslovak Academy of Sciences and sponsored by the International Union of Pure and Applied Chemistry (IUPAC) and the Czechoslovak Chemical Society.

The Microsymposium was attended by 38 foreign and 25 Czechoslovak guests. Five main lectures were presented during the Microsymposium: "New trends in the structure determination of complex organic molecules" (Prof. W. HOPPE); "Computing methods in crystallography" (Prof. J. S. ROLLET); "The structure of amorphous solids" (Dr W. RULAND); "Neutron diffraction studies of organic molecules" (Prof. G. E. BACON); "Optical methods as an aid in structure determination" (Prof. C. A. TAYLOR).

Short communications were divided into the four sections: (a) Structure of low-molecular weight compounds; (b) structure of fibers; (c) disorder in polymers; (d) crystallization of polymers.

The abstracts of short communications were issued for participants. Main lectures are to be published at the official journal of IUPAC "Pure and Applied Chemistry".

**3RD PRAGUE MICROSYMPOSIUM:
DISTRIBUTION ANALYSIS AND FRACTIONATION
OF POLYMERS**

Prague, 23–26 September 1968

The 3rd Microsymposium on Macromolecules took place in Prague (Czechoslovakia). It was organized by the Institute of Macromolecular Chemistry (the Czechoslovak Academy of Sciences) in cooperation with the Institute of Physical Chemistry (the Czechoslovak Academy of Sciences) and the Institute of Physical Chemistry of the Charles University and sponsored by the IUPAC and the Czechoslovak Chemical Society.

The Microsymposium covered the principal problems of both the theory and practice of distribution analysis and fractionation of homopolymers and copolymers. Three main lectures were delivered on the following topics:

- Prof. G. MEYERHOFF (Germany): "Application of the gel chromatography"
- Prof. H. BENOIT (France): "The comparison of different methods for the determination of the polydispersity"
- Dr R. KONINGSVELD (Holland): "Phase relationships and fractionation in multi-component polymer solutions"

26 scientific communications were divided in four sections: (a) Gel permeation chromatography; (b) characterization of polydispersity by physical methods; (c) phase equilibria and fractionation; (d) fractionation of copolymers.

For the participants of the Microsymposium (and for all those interested in) the abstracts of scientific communications were available. The main lectures will be published in the IUPAC journal "Pure and Applied Chemistry" and as a special monograph by Butterworth, London.

**Tentative Specifications for the Measurement and Evaluation
of Infrared Spectra for Documentation Purposes**

Note

At the present time there are about 100000 infrared spectral charts of organic and inorganic compounds on file. The majority of these reside in some half-dozen major collections; there is also one master index which is currently being revised for computer-based search.

The spectra in these collections, for the most part, do not constitute "evaluated data". The individual spectra are of varied technical quality and the compounds are of varied purity and structural validity. There is a need for internationally accepted specifications in order that spectra added to these collections, as well as spectra going into new collections, can be categorized as "evaluated data".

The Commission on Molecular Structure and Spectroscopy has prepared a set of draft specifications that are based on the specifications recommended for Research Quality Analytical Spectra by the Coblenz Society.

The Commission solicits comments on these specifications. They should be sent to the Chairman, Dr R. N. JONES, Division of Pure Chemistry, National Research Council of Canada, Ottawa, Canada. The draft will be reviewed at the XXVth International Conference after which it will be submitted to the Physical Chemistry Division for approval.

1. **Introduction**

These specifications relate to new measurements obtainable on good commercial infrared grating spectrophotometers operated at maximum efficiency under conditions consistent with routine practice in an analytical chemistry laboratory. It is recommended that the spectrum be recorded as a chart or photo-micro chart reproduction. This chart would remain the basic spectral document, but, in addition, a computer-based reference file should be established in which are tabulated all the absorption peak wavenumber positions that are significantly recognizable above the noise level. The band-peak intensities should also be listed in the computer-reference file on an internal relative scale, together with such other information as may later be designated: this might include the elemental analysis data and an internationally recognized compound index number. It is not intended that this computer-storage file would be used directly as a search file. Individual users would be encouraged to prepare their own search programs, adapted to their individual needs.

It must be recognized that all currently available infrared spectrophotometers distort the spectrum to some extent, especially when operated under conditions acceptable in routine laboratory use. These specifications apply only to the absorption spectra of condensed phase systems. It is not considered practical to write specifications for vapor-phase spectra at the present time, nor for emission spectra or reflectance spectra.

1.1 *The evaluating agency*

To be acceptable for documentation purposes as an evaluated spectrum, each curve would need to be approved by a national or international agency designated by CODATA or by one of its participating International Unions for this purpose. Such an organization will be referred to in these specifications as *the evaluating agency*.

At a later date more stringent specifications for a category of "archival" infrared spectra should be established. These would require the recording of the complete contour of the infrared band envelope in computer-readable form. A collection of this type of infrared spectrum would be accumulated slowly and, in the foreseeable future, it would be limited to a comparatively small number of representative compounds.

2. **Specifications**

2.1 *Spectrometer operation*

2.1.1 *Resolution*

The spectral slit width should not exceed 2 cm^{-1} through at least 80% of the wavenumber range, and at no place should it exceed 5 cm^{-1} . There is difficulty in measuring the spectral slit width and its evaluation should be based on comparison with the spectrum of a standard substance, run under the same conditions as were used to produce the submitted spectrum. Indene might be considered a suitable standard substance (see Appendix).

2.1.2 *Wavenumber accuracy*

The abscissal scale, as read from the chart, should be accurate to $\pm 5\text{ cm}^{-1}$ at wavenumbers greater than 2000 cm^{-1} and to $\pm 3\text{ cm}^{-1}$ at wavenumbers less than 2000 cm^{-1} . Calibration corrections within these limits are to be encouraged and should be indicated on the chart.

Proof of the wavenumber accuracy should be an appended spectrum of a standard substance (which could be indene) run under the same conditions as the sample (see Appendix). Fiduciary marks should be recorded on each chart at stated wavenumbers shortly after the beginning, and near or at the end of each uninterruptedly scanned segment of the spectrum. These marks are required to guard against errors from paper shrinkage and from chart-spectrometer mismatch.

2.1.3 *Noise level*

The noise level should not normally exceed 1% average peak-to-peak (or 0.25% rms) through at least 90% of the wavenumber range, but some latitude should be allowed at the discretion of the evaluating agency.

2.1.4 *Energy*

The spectrophotometer should be purged with dry gas or evacuated to ensure that at least 50% of the source energy is available at all wavenumbers. Some latitude may be permitted in the range $2300\text{--}2400\text{ cm}^{-1}$ affected by atmospheric carbon dioxide absorption.

If the control system of the spectrophotometer permits, it is desirable that adequate purging or evacuation be demonstrated by a single beam measurement, or by a mea-

surement against a constant test signal, run under normal scanning conditions with no sample in the beam.

2.1.5 *Other performance criteria*

These are established by reference to the indene or other standard spectrum (see Appendix).

2.1.5.1 *False radiation.* Apparent stray radiation should be less than 2% at wavenumbers greater than 500 cm^{-1} .

2.1.5.2 *Servo system.* The spectrum should exhibit no visual evidence of dead spots or of excessive overshoot. The spectrometer time constant should be compatible with the scan rate (see Appendix).

2.1.5.3 *Photometric accuracy.* These spectra are not intended to have absolute quantitative significance and, at present, it is not feasible to set specifications for photometric accuracy. Such a test, possibly based on the use of rotating sector photometers, might be added later. For the time being it must suffice that the shapes and relative intensities of the bands in the spectrum of the standard substance agree with those of a reference curve acceptable to the evaluating agency.

2.1.5.4 *Sample reradiation.* It is recognized that selective reradiation of energy by the sample can cause error in the absorption measurement, but no specifications for this can be defined at present. Such reradiation constitutes one of the factors that complicate the evaluation of the absolute absorption.

2.1.5.5 *Temperature.* It is to be assumed, unless otherwise stated, that the spectrum is run at the ambient temperature, and some estimate of this temperature (with uncertainty range) should be indicated.

2.2 *Chart presentation*

2.2.1 *Information to appear on the chart*

Both the structural and the molecular formulas of the compound should appear on the chart. It is also recommended that the compound name be included and this should conform with a system of nomenclature approved by the evaluating agency. The make and model of the spectrophotometer should be recorded as well as the date on which the spectrum was obtained. All changes of gratings, filters and cells should be specified, including the wavenumbers at which they occur. No external mechanical attenuator should be placed in the reference beam additional to the small trimmer comb which is an integral component of some commercial infrared spectrophotometers. The name and address of the laboratory contributing the spectrum should be given on the chart.

The physical condition of the sample should be stated (e.g. solution, pure liquid, liquid paraffin mull, potassium bromide pellet matrix, etc.). For measurements on solutions, the solvent used in each region of the spectrum should be recorded. The concentration and nominal path length should be given both for solutions and pellets. The nominal path length of pure liquid samples should also be indicated, but a very thin layer may be described as a "capillary film". The cell or support-window material should be stated.

2.2.2 *Spectral range*

The chart should cover the range 3800 cm^{-1} to 400 cm^{-1} without gaps; extensions above and below this range are acceptable. For such extended range spectra, the wavenumber accuracy, false radiation, atmospheric absorption interference and the spectral slit width should be stated in terms acceptable to the evaluating agency.

2.2.3 *Intensity*

It is preferred that the intensity ordinate values be expressed in absorbance units and that the charts be plotted on paper having a logarithmic ordinate grid so that the intensity in absorbance can be interpolated directly from linear transmittance measurements. Spectra plotted on a linear absorbance scale or in linear transmittance presented on a linear percent transmission ordinate grid are also acceptable.

2.2.4 *Wavenumber readability*

Sharp peaks should be readable from the chart to within 5 cm^{-1} at wavenumbers greater than 2000 cm^{-1} , and to within 2 cm^{-1} at wavenumbers less than 2000 cm^{-1} . Only spectra recorded with the abscissa linear in wavenumber are acceptable, but scale changes at designated abscissal positions are allowed.

2.2.5 *Recording*

Recording should be continuous with no gaps in wavenumber, but it is permissible for spectra to extend over more than one chart. Discontinuities in ordinate, if present, should not exceed 0.01 absorbance unit. Hand-retraced spectra are not acceptable.

Any peak over 1.5 absorbance units must be reproduced on a less absorbing sample. A significant fraction of the useful bands should have absorbance greater than 0.2. At least one band in the spectrum should have absorbance not less than 0.6. When multiple traces are required their number should be kept to a minimum.

2.2.6 *Atmospheric absorption*

None should be detectable (note also Section 2.1.4).

2.3 *Sample identification*

2.3.1 *Compound identity and purity*

Spectra should show no inconsistencies with the postulated structure; any spectrum exhibiting an obvious impurity band should be rejected. Some relaxation of this requirement may be permitted in the case of isotopically labelled substances in which complete isotope exchange cannot reasonably be expected; in such cases the bands associated with the minor isotopic species should be indicated on the chart.

The prime responsibility for the correctness of the designated structure lies with the contributing laboratory and its name and address should be recorded on the chart.

The prime responsibility for the acceptance or rejection of the individual spectrum lies with the evaluating agency.

It is recommended that no spectrum be accepted for documentation unless one or other of the two following criteria can be met:

2.3.1.1 The evaluating agency is supplied with a reasonably detailed description of the preparation and purification history of the measured sample, together with other evidence for the correctness of the assigned chemical structure. This evidence must be sufficient to satisfy an expert in the field.

2.3.1.2 Two curves derived from samples obtained from two independent sources are available; these spectra must be in reasonable agreement.

2.3.2 *Sample preparation*

2.3.2.1 *Liquid state*

2.3.2.1.1 For analytical purposes it is preferable that the sample be run in liquid solution, normally at concentrations in the range of 5 to 10% weight (g) per volume (ml). Solvent bands should be compensated, but not more than 75% of the energy should be removed from the beam by such compensation, and then only over a short spectral region. Any solvent bands resulting from incomplete compensation must be indicated on the chart. A suitable solvent combination is carbon tetrachloride in the range 3800–1335 cm^{-1} and below 650 cm^{-1} and carbon disulfide in the range 1350–430 cm^{-1} ; both solvents should preferably be used at path lengths in the range 0.03–0.3 mm. Cases may arise that require the use of other solvents, and solubility limitations or other concentration dependent factors may necessitate the use of cells of longer path length. These conditions are acceptable provided the requirement of a maximal 75% beam energy attenuation is maintained.

2.3.2.1.2 For documentation purposes it is also desirable that the spectrum of the pure liquid be recorded. Solution spectra and pure liquid spectra are to be regarded as complementary and not as substitutes for one another.

2.3.2.1.3 Liquids not soluble in transparent solvents are to be run as capillary films (see Section 2.2.3).

2.3.2.2 *Solid state*

2.3.2.2.1 For substances that are solid at room temperature, solution spectra in the most transparent solvents are preferred, provided the solvents and path lengths can be chosen to leave no significant gaps due to solvent obscuration (see 2.3.2.1.1).

2.3.2.2.2 For insoluble compounds mulls are preferred to pressed pellets unless it is established that the pellet gives an undistorted spectrum.

Solid state spectra should meet the following criteria:

- *Isotropic materials.* The background absorbance should be less than 0.20 near 3800 cm^{-1} and less than 0.10 near 2000 cm^{-1} . No gross abnormalities should be evident in the background. Compensation in the reference beam by a blank mull or pellet, if present, should be indicated, and in no case should it reduce the reference radiation intensity by more than 50%. The Christiansen effect should not be apparent, but minor distortion resulting from this effect may be permitted at the discretion of the evaluating agency. Interference fringes should not be apparent. Pellets should exhibit no water absorption bands greater than 0.03 absorbance unit. Mulls should be made with perhalogenated oils (or their spectroscopic equivalent) for the range 3800–1335 cm^{-1} and the intensity of the overtone band near 2300 cm^{-1}

should not exceed 0.02 absorbance unit. A liquid petroleum mulling agent should be used below 1335 cm^{-1} and the intensity of the band near 720 cm^{-1} should not exceed 0.05 absorbance unit.

- *Nonisotropic materials.* Spectra of nonisotropic materials, such as single crystals or crystalline polymer films should also be accompanied by a record of the orientation of the sample with respect both to the radiation beam and to the grating rulings.

Amorphous and partially crystalline polymers of ill-defined molecular or conformational structure should not be included as pure materials.

APPENDIX

1. Spectrophotometer Performance Checks

The recommended performance checks are based on a set of measurements carried out on a standard material determined close in time to the sample-spectra measurements and submitted to the evaluating agency. The checks described below use a test material composed of a ternary mixture of indene, camphor and cyclohexanone, but alternative standards might be considered subject to the approval of the evaluating agency.

1.1 Wavenumber calibration

For the range $3800\text{--}700\text{ cm}^{-1}$ the wavenumber calibration should be checked on a sample of indene containing 0.8% (by weight) of cyclohexanone and 0.8% (by weight) of camphor. This solution, prepared from freshly distilled indene and cyclohexanone, and freshly sublimed camphor, should be stored in sealed glass ampoules opened just before use. The spectrum is published in “Tables of Wavenumbers for the Calibration of Infrared Spectrometers” [2], see also reference [3].

Below 700 cm^{-1} a solution prepared from equal parts (by weight) of indene, camphor and cyclohexanone can be used [4] pending the establishment of approved standards for this spectral range.

Each set of spectra should be accompanied by a set of test spectra run significantly closely in time to the submitted spectra and measured at the same slit width, noise level, scanning speed and time constant. A nominal cell thickness of 0.2 mm is recommended for the range $3800\text{--}1580\text{ cm}^{-1}$ and 0.03 mm for the range $1600\text{--}700\text{ cm}^{-1}$. A cell thickness of 0.05 mm is recommended for the 1:1:1 mixture used below 700 cm^{-1} . The recommended calibration points (cm^{-1}) are the absorption maxima listed in Table I.

Table I Absorption maxima recommended for calibration of the wavenumber scale (cm^{-1})

Solution I

3927.2	3798.9	3660.6	3297.8	3139.5	2770.9	2598.4
2305.1	2090.2	1915.3	1797.7	1741.9	1713.4	1661.8
1587.5	1361.1	1312.4	1288.0	1226.2	1205.1	1122.4
1067.7	1018.5	914.7	830.5	730.3		

Solution II

693.0 647.5 551.5 489.0 381.5

Solution I [indene 98.4 %, cyclohexanone 0.8 %, camphor 0.8 % (by weight)]

Solution II [indene 33.3 %, cyclohexanone 33.3 %, camphor 33.3 % (by weight)]

1.2 *Dynamic error*

The following dynamic error test is suitable for use with most spectrophotometers. The indene spectrum is rerun from 1350 to 850 cm^{-1} at one fourth of the scanning rate used for the reference spectra, with the other operating conditions unchanged. The heights from the baseline of the bands at 1288.0, 1226.2, 1205.1, 1018.5 and 914.7 cm^{-1} are measured in absorbance units on both the fast and slowly scanned charts. The peak-height ratios $A_{1288.0}/A_{1226.2}$, $A_{1205.1}/A_{1226.2}$ and $A_{1018.5}/A_{914.7}$ should not differ by more than ± 0.02 between the fast and slow scans.

1.3 *Spectral slit width*

This quantity can be determined approximately in the neighbourhood of 1200 cm^{-1} from the ratio $A_{1205.1}/A_{1226.2}$ which is evaluated in the dynamic error test, namely:

$A_{1205.1}/A_{1226.2}$	Approximate spectral slit width (cm^{-1})
0.80	4.0–5.0
0.85	3.0–3.5
0.90	2.0–2.5
0.95	1.0–1.5
0.97	< 1.0

1.4 *False radiation*

The indene spectrum should have negligible transmission at 3050.0, 1609.6 and 765.4 cm^{-1} if measured at the designated thicknesses. The test spectra at these wavenumbers should therefore match the spectrometer transmission zero within the allowed tolerances (see Section 2.1.5.1). A 0.4-mm layer of indene is totally absorbing at 551, 420 and 392 cm^{-1} and this may be used to evaluate the false radiation below 600 cm^{-1} .

1.5 *Photometric accuracy*

See Section 2.1.5.3.

1.6 *Check on I_0*

Each set of spectra should be accompanied by an I_0 check obtained by scanning the wavenumber range of the submitted spectra with no cell in either beam at the same slit width, noise level, scanning speed and recorder time constant. The I_0 trace should lie within a range of ± 0.01 absorbance units.

1.7 *Cell blank check*

Each set of solution spectra should be accompanied by a chart trace obtained at the same slit width, noise level, scanning speed and recorder time constant, with solvent in both cells, using the same cells as for the submitted spectra. No extraneous bands should appear, though it is recognized that solvent bands may not be completely compensated in the cell-blank spectrum. The degree of allowable mismatch is left to the discretion of the evaluating agency.

See Section 2.1.4.

References

- 1 *Analytical Chemistry* 38, 27A (1966)
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- 3 R. N. JONES/A. NADEAU. *Spectrochim. Acta* 20, 1175 (1964)
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24 November 1968

REVISION OF RED BOOK: NOMENCLATURE FOR BERTHOLLIDES*

9. Crystalline Phases of Variable Composition

Compounds involving isomorphous replacement, interstitial solutions, inter-metallic compounds, semiconductors and other nonstoichiometric compounds (berthollides)

9.11 If an intermediate crystalline phase (whether equilibrium phase or not) occurs in a two-component (or more complex) system, it may obey the law of constant composition with a very high accuracy, as in the case of sodium chloride, or it may be capable of varying in composition over an appreciable range, as occurs for example with FeS. A substance showing such a variation is called a *berthollide*.

In connection with the berthollides the concept of a characteristic or ideal composition is frequently used. A unique definition of this concept seems to be lacking, but usually the definition is based upon the crystal structure. Sometimes one can state several characteristic compositions. In spite of this the concept of a characteristic composition can be used when establishing a system of notation for phases of variable composition. It is also possible to use the concept even if the characteristic composition is not included in the known homogeneity range of the phase.

9.12 For the present, formulae should preferably be used for berthollides and solid solutions, since strictly logical names tend to become inconveniently cumbersome. The latter should only be used when unavoidable (*e.g.*, for indexing), and may be made in the style of: iron(II) sulfide (iron deficient); molybdenum dicarbide (excess carbon), or the like. Mineralogical names should only be used to designate actual minerals and not to define chemical composition; thus the name calcite refers to a particular mineral (contrasted with other minerals of similar composition) and is not a term for the chemical compound whose composition is properly expressed by the name calcium carbonate. (The mineral name may, however, be used to indicate the structure type, see 6.52.)

Formulae should be based on structural units and not on analytical ratios of elements.

9.21 Various notations are used for the berthollides, depending upon how much information is to be conveyed.

A general notation, which can be used even when the mechanism of the variation in composition is unknown, is to put the sign \sim (read as *circa*) before the formula. (In special cases it may also be printed above the formula.)

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Examples



If it is desirable to give more information, one of the following notations may be used.

9.22 For a phase where the variable composition is solely or partially caused by replacement, atoms or atomic groups which replace each other are separated by a comma and placed together between parentheses.

If possible the formula ought to be written so that the limits of the homogeneity range are represented when one or other of the two atoms or groups is lacking. For example the symbol (Ni,Cu) denotes the complete range from pure Ni to pure Cu; likewise K(Br,Cl) comprises the range from pure KBr to pure KCl. If only part of the homogeneity range is referred to, the major constituent should be placed first.

Substitution accompanied by the appearance of vacant positions (combination of substitutional and interstitial solution) may receive an analogous notation. For example (Li₂,Mg)Cl₂ denotes the homogeneous phase from LiCl to MgCl₂. The formula (Mg₃,Al₂)Al₆O₁₂ represents the homogeneous phase from the spinel MgAl₂O₄ (= Mg₃Al₆O₁₂) to the spinel form of Al₂O₃ (= Al₂Al₆O₁₂).

9.23 A more complete notation, which should always be used in more complex cases, may be constructed by indicating in a formula the variables which define the composition. Thus, a phase involving simple substitution atom for atom of A for B may be written A_{m+x}B_{n-x}C_p.

Examples

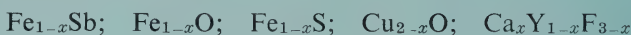


In the case of the γ -phase of the Ag-Cd-system, which has the characteristic formula Ag₅Cd₈, the Ag and Cd atoms can replace one another to some extent and the notation would be Ag_{5±x}Cd_{8∓x}. For the plagioclases the notation will be Na_xCa_{1-x}Al_{2-x}Si_{2+x}O₈ or Na_{1-y}Ca_yAl_{1+y}Si_{3-y}O₈. This shows immediately that the total number of atoms in the unit cell is constant.

The commas and parentheses called for in 9.22 are not required in this case.

Interstitial or subtractive solution, whether combined with substitutional solution or not, can be shown in an analogous way. For example, the homogeneous phase between LiCl and MgCl₂ becomes Li_{2x}Mg_{1-x}Cl₂, showing that the anion lattice remains the same but that one vacant cation position appears for every replacement of 2Li⁺ by Mg²⁺. The phase between MgAl₂O₄ and Al₂O₃ can be written Mg_{3x}Al_{2(1-x)}Al₆O₁₂ which shows that it cannot contain more Mg than that corresponding to MgAl₂O₄ (x = 1).

Further examples



Na_{1-x}WO₃ or Na_yWO₃ (sodium tungsten bronzes, depending on the choice of characteristic composition).

For $x = 0$ each of these formulae corresponds to a characteristic composition. If it is desired to show that the variable denoted by x can only attain small values, this may be done by substituting δ or ε for x .

When using this notation, a particular composition can be indicated by stating the actual value of the variable x . Probably the best way of doing this is to put the value in parentheses after the general formula. For example, $\text{Li}_{4-x}\text{Fe}_{3x}\text{Ti}_{2(1-x)}\text{O}_6$ ($x = 0.35$). If it is desired to introduce the value of x into the formula itself, the substitution is more clearly understood if one writes $\text{Li}_{4-0.35}\text{Fe}_{3 \times 0.35}\text{Ti}_{2(1-0.35)}\text{O}_6$ instead of $\text{Li}_{3.65}\text{Fe}_{1.05}\text{Ti}_{1.30}\text{O}_6$.

The solid solution of hydrogen in palladium can be written as PdH_x ($x < 0.1$) and the palladium hydride phase as PdH_x ($0.5 < x < 0.7$). A phase of the composition M which has dissolved a variable amount of water can be written $M(\text{H}_2\text{O})_x$.

9.31 If in addition to the chemical composition the existence of vacant sites and interstitial sites is to be shown, this can be done by using additional symbols as indicated in 9.311–9.314.

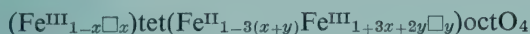
9.311 A site in the structure of the ideal composition is represented by the square, \square , and an interstitial site by the triangle, Δ . Where it must be shown if a site is cationic or anionic, a cationic site is shown by \square_{cat} and an anionic site by \square_{an} . Crystallographically different sites can be distinguished by adscripts, *e.g.* \square_a , \square_b , or \square_{tet} , \square_{oct} , the two last adscripts denoting tetrahedral or octahedral sites. A more precise notation could be obtained by putting in brackets immediately after the site symbol the point group symbol showing the symmetry of the nearest environment of the site and its coordination number, *e.g.* $\square[\text{O}_h; 6]$.

9.312 An atom A in the site \square is expressed by the symbol $(A|\square)$. Spinel can thus be represented by $(\text{Mg}|\square_{\text{tet}})(\text{Al}|\square_{\text{oct}})_2\text{O}_4$, Mg being situated in tetrahedral and Al in octahedral sites formed by the oxygen atoms. The “inverse spinel” magnetite is represented by $(\text{Fe}^{\text{III}}|\square_{\text{tet}})(\text{Fe}^{\text{II}}_{\frac{1}{2}}\text{Fe}^{\text{III}}_{\frac{1}{2}}|\square_{\text{oct}})_2\text{O}_4$, which means that Fe^{II} and half of the Fe^{III} are distributed at random over certain octahedral sites.

9.313 If n atoms A are distributed over m sites \square , this is expressed by $(A_n|\square_m)$. This implies that $m-n$ sites are vacant, and it is not necessary to show them specially. The γ -modification of Fe_2O_3 is thus $(\text{Fe}^{\text{III}}_{8/3}|\square_3)\text{O}_4$. Using this notation we can write the lithium magnesium chloride as $(\text{Li}_{2x}, \text{Mg}_{1-x}|\square_2)\text{Cl}_2$.

9.314 A vacant site is represented by the single symbol \square , without atomic symbol. The vacant position in lithium magnesium chloride can thus be shown as $\text{Li}_{2x}\text{Mg}_{1-x}\square_{1-x}\text{Cl}_2$ or $\text{Li}_{1-2y}\text{Mg}_y\square_y\text{Cl}$.

Some authors find the symbols given in 9.312 and 9.313 unnecessary. We can write the spinel formula $\text{Mg}^{\text{II}}_{\text{tet}}\text{Al}^{\text{III}}_{\text{oct}}\text{O}_4$ and the inverse spinel type magnetite $\text{Fe}^{\text{III}}_{\text{tet}}(\text{Fe}^{\text{II}}\text{Fe}^{\text{III}})_{\text{oct}}\text{O}_4$. Maghemite ($\gamma\text{-Fe}_2\text{O}_3$) is $(\text{Fe}_{1-x}\square_x)_{\text{tet}}(\text{Fe}_{2-y}\square_y)_{\text{oct}}\text{O}_4$, with $x + y = 1/3$, where x and y can be determined by X-ray diffraction methods. Intermediates between magnetite and maghemite are found in nature; they can be written



A heated potassium chloride crystal with Schottky defects (cation vacancies *and* anion vacancies) can be written $(\text{K}_{1-\delta}\square_{\delta})(\text{Cl}_{1-\delta}\square_{\delta})$.

A silver bromide crystal with Frenkel defects (cation vacancies *and* interstitial cations, but with the anion lattice intact) is written $(\text{Ag}_{1-\delta}\square\delta)(\text{Ag}\delta|\Delta)\text{Br}$. Although the sign $|\Delta$ could be left out, it improves clarity.

The α -modification of silver iodide, where the cations are distributed at random over cation sites *and* interstitial sites, can be written $(\text{Ag}|\square, \Delta)\text{I}$.

9.32 In the discussion of catalytic reactions designation of a site in the surface by \square_{surf} is useful. An interstitial site in the surface will be Δ_{surf} . An oxide ion in the surface of a metal oxide will then be designated by $(\text{O}^{2-}|\square_{\text{surf}})$. The type of surface site occupied is specified as in the example $(\text{O}^{2-}|\square_{\text{oct, surf}})$, where the oxide ion occupies a potentially octahedral site.

9.33 Electrons and positive holes bound in the field of an excess positive or negative charge are designated by “e⁻” and “p⁺” respectively.

Examples: Germanium doped with arsenic or gallium is $\text{Ge}_{1-\delta}\text{As}\delta$ or $\text{Ge}_{1-\delta}\text{Ga}\delta$ respectively, but if it is desired to emphasize the semiconductor properties this can be expressed by the formulae $\text{Ge}_{1-\delta}\text{As}^+\delta\text{e}^-\delta$ or $\text{Ge}_{1-\delta}\text{Ga}^-\delta\text{p}^+\delta$, although it is known that no more than 50% of the impurity atoms are ionized at room temperature.

Likewise sodium chloride with excess sodium has anion vacancies (F-centres) expressed by $\text{Na}^+\text{Cl}_{1-\delta}\text{e}^-\delta$, or, if it is desired to show that the electron is trapped in an anion vacancy $\text{Na}^+(\text{Cl}_{1-\delta}\text{e}^-\delta|\square_{\text{an}})$.

Zinc oxide with excess zinc is on the contrary believed to contain interstitial cations (and electrons trapped by them), expressed by $(\text{Zn}^{2+}|\square)(\text{Zn}^{2+\delta}\text{e}^{-2\delta}|\Delta)\text{O}^{2-}$.

9.34 To indicate that two kinds of defect occur in association the symbol χ may be used.

Example Iron-deficient iron(II)oxide $\text{Fe}^{\text{II}}_{1-3x}\text{Fe}^{\text{III}}_{2x}|\Delta\chi|\square_{\text{cat}3x}\text{O}$.

Note:

A different system for designating imperfections in crystals is given by F. A. KRÖGER: *The Chemistry of Imperfect Crystals*. Amsterdam 1964, p. 1001–1002.

Authors in the semiconductor field use n and p for electrons and positive holes respectively, but these letters are also widely used to designate neutrons and protons respectively.

VI.5.1 IUPAC COMMISSION ON TERMINAL RESIDUES

By H. EGAN, Secretary to the Commission

The Third Meetings of the Terminal Residues Commission of the Pesticide Section of the Applied Chemistry Division of IUPAC were held in Sittingbourne, Kent, England, in October 1968, under the chairmanship of Dr H. HURTIG. The following account of the proceedings is based on the minutes of the meeting and on the appendixes drawn up by members and associate members of the Commission as indicated. The Commission considered the report of the Joint FAO/WHO Meeting on Pesticide Residues held in Rome in December 1967 in which some problems concerning terminal residues were discussed. These problems were assigned by FAO/WHO; their solution would ultimately be of use to the FAO/WHO Codex Alimentarius Commission.

1. Terminal lindane residues

The Commission recognized the need for further information on the nature of the terminal residues arising from the agricultural (as opposed to the veterinary) uses of lindane and reviewed work on this in progress in Canada, Germany, Japan, the Netherlands and the United States. MORLEY [1] had shown the formation of gamma-pentachlorocyclohexene in soil treatments. Arrangements were made for reporting further progress.

2. Terminal cyclodiene residues

The Commission reviewed work in progress on the elucidation of terminal residues arising from the use of cyclodiene insecticides, with particular reference to the role played by microsomal enzyme systems in biotransformation, to environmental transformations resulting from the action of micro-organisms or exposure to sunlight and to plant-soil interactions. Arrangements were made to continue the co-ordination of this information; and in particular, to collate information on the fate of organochlorine pesticide residues in processing edible oils.

2.1 Evaluation

2.1.1 General degradation studies—by P. E. PORTER

Although there is little immediate advance in knowledge of the terminal residues of cyclodiene insecticides, much work is in progress in many parts of the world and considerable clarification of the position can be expected in the near future. TERRIER [2] has surveyed the literature on microsomal enzyme studies, and is examining the properties of systems isolated from rats, trout, quail and insects. Other workers in this field include MATTHEWS and MATSUMURA [3] and BROOKS and HARRISON [4]. A similar situation exists in animal metabolism studies and the reverse transformation in resistant mosquitoes, from dieldrin to aldrin, has been confirmed by TOMLIN [5]. MATSUMURA and BOUSCH [6] have recognized dieldrin degrading organisms in selected soils but products have not yet been fully identified. A number of workers are studying the uptake by plants of cyclodienes from soil but a full clarification of the position is not yet possible. RICHARDSON [7] and KIIGEMAGI [8] have indicated that saponification as an analytical clean-up procedure for animal tissues may itself result in some degradation of dieldrin.

Experiments in which surface leaf applications of ^{14}C endrin were made to cabbage, tobacco and carrots have indicated that losses are due mainly to volatilization; the same is true of aldrin and dieldrin loss from soils [9]. Hydrophilic metabolites also occur however, and in cabbage the levels found after four weeks increased in the sequence leaves, stalks, roots, soil, the concentration of radioactivity decreasing in the same sequence. A similar picture was found with carrots [10]. In order to prove that the hydrophilic products really were metabolites, and not compounds formed by the action of air and light in active surfaces, control experiments were carried out using dead leaves, glass plates, thin silica layers and plant homogenates. Conversion did not exceed 2% in any of these experiments, compared with 14% on cabbage plants kept in the dark. Work is continuing with aldrin and other cyclodienes, the general indication being that plants do in fact metabolize drin insecticides; endrin is metabolized more easily by animals than by plants, the reverse is true for aldrin, whilst the ease of conversion for dieldrin is similar in plants and animals.

3. **Terminal chlordane residues**

The Commission considered further progress in the understanding of the influence of climatic conditions, and of subsequent cooking or other processing operations, on the nature and extent of residues arising from the use of chlordane. Results from field studies on beans and cabbage in six countries in Europe and North America showed that in general climatic conditions do not affect the compositions or level of residues significantly except that in the northernmost location (Finland) a slower rate of disappearance than the average was found. Simple cooking has little influence on the residues but some losses occur in dried milk production and substantial losses were indicated in edible oil processing. Arrangements were made to extend these studies to other vegetable crops; and also to review the general validity or otherwise of the concept of residue “half lives”.

3.1 *Evaluation*—by P. B. POLEN

In a search for the quantitative regional influences and the effects of cooking upon chlordane residues, a study has been completed for foliar applications to beans and cabbages in seven locations within Europe and North America. The results indicate that climatic conditions do not significantly influence the composition, pattern of dissipation or levels of residues when compared with other experimental variables [11]. Simple cooking of the beans or cabbage by boiling for 10 minutes in salted water also had no significant effect on levels or composition of the residues. For milk, processing operations as in condensed milk, dried milk or evaporated milk production reduce the residues by from 25 to 50% [12]. The earlier work of GOODING [13] has been supported by further evidence that the processing of edible vegetable oils under commercial conditions removes residues of several pesticides, including chlordane [14]. Studies are in progress to determine the identity of the separate metabolites which arise from alpha- and gamma-chlordane isomers; these have gas chromatographic characteristics similar to those of heptachlor epoxide but neither is identical with this.

4. Terminal carbamate residues

The Commission reviewed progress in the knowledge of terminal residues arising from the use of carbaryl and other carbamate insecticides, including Temik, carbofuran and Mobam (4-benzothienyl methylcarbamate). The formation of 5, 6-dihydro-5, 6-dihydroxy carbamates is now well established but further work is required to establish whether the aglycones formed in plants correspond to the glucuronides in animal metabolism and on the nature of residues resulting from foliar application to plants.

4.1 *Evaluation*—by J. W. COOK and G. L. SUTHERLAND, assisted by R. BARON
The identity of the major oxidative metabolite of carbaryl has been confirmed as a glycoside of the methylcarbamate ester of 5,6-dihydro-5,6-dihydroxy-1-naphthol [15]. BARON *et al.* [16], using a metabolite isolated from the urine of a carbaryl treated cow, found that the metabolite was not detected by standard colorimetric techniques although under certain conditions it could be converted to compounds which could be detected. Limited toxicological studies indicated that the compound was less toxic than carbaryl and not mutagenic. The occurrence of a potential metabolite, the methylcarbamate of 3, 4-dihydro-3, 4-dihydroxy-1-naphthol was not discussed. DOROUGH and WIGGINS [17] have evaluated the analytical colorimetric techniques for determining the plant residues using stem injection techniques and have investigated the fate of these residues in rats. DOROUGH [18] and BARON *et al.* [19] studied residues in milk resulting from oral administration of carbaryl to lactating cow. Using carbonyl-labeled carbaryl residues 3 times higher than those using naphthyl-labeled carbaryl were observed. In each case carbaryl residues were not detectable colorimetrically. BARON [20] further investigating the apparent disparity in residue resulting from similar treatments observed that the major water-soluble radioactive residue consisted of ^{14}C lactose.

Plant and animal metabolic studies with other methylcarbamate insecticides have been extensive in 1968 and again reflect similar patterns of oxidation and/or hydrolysis followed by conjugation and either elimination (insects and mammals) or storage (plants). Studies on the fate of Temik (2-methyl-2-(methylthio) propionaldehyde O-(methylcarbamoyl) oxime) have been extended to include insects [21], milk [22, 23], plants and soil [24], and rats [25]. The initial metabolism studies in the 1967 report have been confirmed. In all known biological systems the major metabolic pathway for Temik is rapid oxidation to Temik sulfoxide and a slower subsequent oxidation to Temik sulfone. Both carbamates are degraded further to oximes and nitriles.

Plants degrade Temik in a manner which closely parallels the mammalian metabolic pathways. Incorporated into the cotton plants by injection or soil uptake, Temik is largely metabolized after one week. The primary metabolite, Temik sulfoxide, is slowly oxidized to the less toxic Temik sulfone. The ratio of Temik sulfoxide to Temik sulfone in cotton leaves changed over a six-week period from 15:1 to 1:1. The half-life of Temik in soil under field conditions is less than one week. Soil micro-organisms are not affected by Temik or its metabolites and in several cases studied appear to metabolize the pesticide effectively. The persistence and toxicity of the sulfoxide are especially noteworthy.

The metabolic fate of carbofuran in milk [26, 27, 28] rats and insects [29] and plants [30, 31] confirms the oxidative formation of the 3-hydroxy metabolite and the corre-

sponding keto metabolite. The plant conjugates, presumably glycosides, may be hydrolyzed following ingestion to aglycones and reconstituted as glucuronides before elimination. Preliminary studies on the metabolism of Mobam (MCA-600, 4-benzothienyl N-methylcarbamate) in barley and alfalfa [32] and rats [33] have again demonstrated that the major metabolites were conjugates of the 4-benzothienyl hydrolytic moiety. In a manner similar to that reported for carbaryl in 1967, Mobam was readily translocated upward in the xylem of barley and alfalfa grown in nutrient solution containing the carbamate. A preliminary report on the metabolism of Landrin (3, 4, 5- and 2, 3, 5-trimethylphenyl N-methylcarbamates), following injection into bean plants, indicated that the compounds were oxidized at several positions on the molecule [34].

5. **Terminal organophosphorus compound residues**

The Commission considered progress in the knowledge of the nature of terminal residues arising from the use of diazinon and dimethoate and made arrangements for assessing the adequacy of analytical methods for residues of organophosphorus pesticides in general and total diet studies.

5.1 *Evaluation*—by E. Y. SPENCER and G. L. SUTHERLAND

5.1.1 *Diazinon*

In excised leaf and root absorption studies of ^{14}C -labeled diazinon with bean plants, the only chloroform-soluble metabolites were the parent compound and its pyrimidinol hydrolysis product [35]. In leaves the pyrimidinol constituted virtually all of the chloroform-soluble radioactivity, a negligible amount of which was converted to radioactive carbon dioxide. In contrast to the foliar application studies of RALLS [36] no oxygen analog was isolated as a result of the present methods of application. Recent work has indicated a previously unreported cholinesterase inhibitor isolated from field sprayed kale [37]. It has been tentatively identified as hydroxy diazinon, similar to the product isolated after UV irradiation.

Eighteen dimethoate metabolites from bean plants have been isolated in a study of the mode of application of the insecticide [38]. Those identified were des-N-methyl, oxygen analog, dimethoate carboxylic acid, des-O-methyl, des-O-methyl carboxylic acid, O, O-dimethyl phosphorothioic acid and O, O-dimethyl phosphorodithioic acid. Two incompletely identified metabolites, possibly N-hydroxymethyl derivatives of dimethoate and its oxygen analog, were isolated from the foliar application only, and, while comprising about 10% of the initial dose at two days, had disappeared by four days. A fine review of dimethoate metabolism has recently been published [39].

6. **Terminal dithiocarbamate residues**

The Commission received brief details of a few publications on recent work on the nature of terminal residues arising from the use of dithiocarbamate fungicides and made arrangements for the future collation and co-ordination of information in this field.

7. **Terminal fumigant residues**

The Commission reviewed progress on the knowledge of the nature of terminal residues and reaction products with food arising from the use of fumigants, with particular reference to the fact that information on the latter was still relatively small.

7.1.1 Terminal residues—by E. E. KENAGA and J. W. COOK

Ethylene oxide (EO) has been shown to leave residues of ethylene glycol (EG) and diethylene glycol in fumigated foodstuffs. EO will react with moisture to form EG and with sugars to form glycol derivatives. Proteins react with EO at several sites on the molecule to form the corresponding hydroxethyl compounds.

In 1965, WESLEY *et al.* [40] showed that foodstuffs heavily fumigated with 750 ml EO/m³ for five hours gave ethylene chlorohydrin (ECH) residues of 1 ppm in dried peas up to 260 ppm in flour and 310 ppm in spray-dried albumin. EO will combine with chlorine derived from small amounts of inorganic chlorine to form ECH. Chloride availability is seldom a limiting factor. HEUSER and SCUDAMORE [41, 42] discuss the problems of avoiding breakdown of EO to ECH in the extraction procedure during analysis and the difficulties of extracting ECH. An improved extraction procedure using a water-acetone solution proved 98% effective in recovering ECH.

Propylene oxide (PO) has been shown to leave residues of propylene glycol (PG) by reaction with moisture in fumigated foodstuffs. Propylene oxide can also react with sugars to form glycol derivatives. The analytical method for PG is sensitive to about 1 ppm [41]. WESLEY *et al.* [40] have shown that under fumigating conditions PO will combine with small amounts of inorganic chlorides to form propylene chlorohydrin (PCH).

RAGELIS *et al.* [43, 44] used gas chromatographic and infrared spectrophotometry techniques and various isolation methods (steam distillation and sweep codistillation) in conjunction with the ether extraction method to analyze for PCH. Two types of PCH were found in various food products treated with PO, mainly 1-chloro-2-propanol and possibly 2-chloro-1-propanol.

MUNRO and MORRISON [45] found that extraction of lyophilized cod fillets with 1, 2-dichloroethane (EDC) resulted in reaction with trimethyl amine and formation of chlorocholine chloride (CCC) ((2-chloroethyl) trimethyl ammonium chloride), a toxic choline derivative. The formation of this choline derivative is unique to EDC-treated fish protein and results from conditions of high temperatures and concentrations of EDC in intimate liquid contact with fish. Such a derivative probably would not be formed in fumigated grain and grain products. Comparisons of the chemical structures of residues in freeze-dried cod fillets after similar drastic extraction conditions with synthetic chemical standards suggested that sulfohydryl groups of proteins can be alkylated to produce thioether linkages such as S, S'-ethylenebiscysteine (MORRISON and MUNRO [46]). It is not believed that such conditions occur in the fumigation of commodities under normal fumigation conditions.

7.1.2 Reaction products with food—by J. W. COOK, assisted by M. PEREZ

BERCK has reviewed the subject of fumigant reactivity [47]. A wide spectrum of evidence has been given to show the possibility that various mechanisms of reactivity might occur providing potential harm to man and animals. However, in any clearly definitive investigations of which there are few, where an attempt was made to identify the nature and quantitate the amount of reaction products formed under conditions simulating normal fumigation practices, no threat to man's health has been identified. Additional work reported since 1964 has for the most part lent support

to the hypothesis that a potential problem may exist, but again these investigations have not been sufficiently germane in design to evaluate in a practical sense what actually occurs when foodstuffs were subject to normal fumigation. The most comprehensive and definitive studies reported were by WINTERINGHAM *et al.* [48] and BRIDGES [49] in 1955 using ^{14}C -labeled methyl bromide in the fumigation of whole wheat flour and wheat gluten of 5 and 15% moisture content with subsequent aeration. The gluten or protein fraction of the flour was responsible for 80% of the decomposition of absorbed fumigant primarily due to methylation with the formation of 50% of N-methyl, 30% of dimethylsulphonium and 20% of methoxyl and thiomethoxyl derivatives in about equal proportions. Similar results were obtained when gluten alone was exposed to the labeled fumigant, with a decrease in decomposition with increased moisture content. The N-methylation was shown highly selective with basic amino acids. The predominant reaction products were characterized by BRIDGES as 1-N-methyl, 3-N-methyl and 1,3-N-dimethyl histidines. Under conditions of fumigation which were more vigorous than necessary to destroy insects, BRIDGES estimates that only about 4.5% of the total histidine content of the flour was involved in the reactions assuming only monomethylation occurred. LEWIS [50] observed that when methyl bromide was added to several enzyme systems dependent on essential —SH groups, irreversible enzyme inhibitions occurred. The addition of methyl bromide to cysteine and reduced glutathione resulted in a decrease in —SH and an increase in nonvolatile bromide. Methyl bromide fumigation has resulted in obnoxious odours in such diverse products as tobacco, beans, and various bakery products. Complete destruction of the reactive thiol group of glutathione was obtained on treatment with methyl bromide, chloropicrin, trichloroacetonitrile and ethylene oxide, and partial destruction by methyl chloride, methyl iodide, ammonia and carbon disulfide [51].

^{82}Br -labeled ethylene dibromide was used by BRIDGES [52] to study the absorption and decomposition of wheat. The amount of chemical reaction was found to be small at room temperature compared to methyl bromide. Ethylene glycol formed when imperfectly aired fumigated wheat was heated. SINCLAIR *et al.* in 1962 [53] studied the sorption of ethylene dibromide on a number of fruits. In addition he added 2.6–7.9 mg of ethylene dibromide to macerated tissues of avocados, oranges, and lemons and after storage at room temperature for 10 days determined the residue of the parent compound. From the high percent recoveries of ethylene dibromide ranging from 84% for lemons to 95% for avocados he concluded that ethylene dibromide was quite stable and unreactive with fruits.

Moisture readily opens the epoxide ring of ethylene and propylene oxide to form corresponding glycols. GORDON *et al.* [54] has shown that the fumigation of dried prunes with ^{14}C -labeled ethylene oxide results in 50% of the total radioactivity as insoluble hydroxyethyl cellulose in the prune skin, 30% in the pulp as hydroxyethylated sugars, 3% as glycols mainly ethylene glycol and the remainder as hydroxyethylated amino acids and proteins. PAGE [55] treated dried fruit with HCN and found evidence that levulose cyanohydrin may be formed. Sulfur dioxide used as a preservative treatment for fruits was found by BURROUGHS and SPARKS [56] to react with ketones and carbonyls to form bisulfite addition products.

8. Terminal methylenedioxyphenyl synergist residues

The Commission received a report on progress in the knowledge of terminal residues arising from the use of methylenedioxyphenyl synergists and on recent work on the effect of piperonyl butoxide on the stability of pyrethrum extracts.

8.1 Evaluation—by J. B. MOORE

A study of the metabolism by mice of methylenedioxyphenyl compounds by KAMIENSKI and CASIDA [57] shows the effect of microsomal-NADPH enzyme systems on these compounds. These drugs or insecticides are metabolized almost exclusively by the microsomal-NADPH enzyme system.

HEAD *et al.* [58] in a study on the effect of piperonyl butoxide on the stability of films of pyrethrum extract, studied the structure of the degraded pyrethrum products. The observations of the retention times on modification of the structure indicated that in the breakdown of pyrethrins, cinerin and jasmolin, the mode of breakdown was the same for all molecules and indicated that the attack was on the chrysanthemumic and pyrethric acid moiety and that the alcohol portion of the molecule remained unchanged. They found the same thing in the case of allethrin. These breakdown products have not yet been identified.

CHEN and CASIDA [59] in a study of photodecomposition found that "on exposure to air and light as residual films, pyrethroids convert to polar products, generally without ester hydrolysis. Studies with ^{14}C -labeled preparations of allethrin, dimethrin, phthalthrin, and pyrethrin I partially define the nature of the reactions occurring on the *trans*-chrysanthemumate moiety photodecomposition. Pyrethrin I decomposes most rapidly, allethrin and phthalthrin degrade at intermediate rates, and dimethrin is the most volatile and least photolabile of the esters studied. Many photodecomposition products form in each case and, at least with allethrin and phthalthrin, the products are esters because the same ones are detected with both acid- and alcohol-labeled preparations. Allethrin is modified by light on the alcohol moiety, based on studies with the alcohol-labeled preparation. Chrysanthemumic acid is not one of the ten or more acids recovered on saponification of the photodecomposed, acid-labeled pyrethroids. Among these acids, *trans*- and meso-*cis*-caronic acids are identified by co-chromatography. Thus, oxidative cleavage of the double bond and *trans-cis* isomerization occurs on photodecomposition of each of the pyrethroids. Other acids formed on photodecomposition appear to be, in part, the same ones resulting from the attack of potassium permanganate on chrysanthemumic acid or on the acid moiety of allethrin."

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**VI.5.2 REPORT OF THE IUPAC COMMISSION
ON THE DEVELOPMENT, IMPROVEMENT, AND STANDARDI-
ZATION OF METHODS OF PESTICIDE RESIDUE ANALYSIS**

By H. EGAN, Secretary to the Commission

The Third Meetings of the Residue Analysis Commission of the Pesticides Section of the Applied Chemistry Division of IUPAC were held in Sittingbourne, Kent, England, in October 1968, under the chairmanship of Dr R.A.E. GALLEY. The following account of the proceedings is based on the minutes of the meeting and on the appendices presented by the members and associate members of the Commission as indicated. The Commission considered the report of the Joint FAO/WHO Meeting on Pesticide Residues held in Rome in December 1967 in which some problems concerning residue analysis were discussed. The Commission noted that the Codex Alimentarius interests in analysis related to methods of international referee status, and expressed the view that equivalence between two or more such methods could be assessed only insofar as the methods were acceptable (as opposed to equal or identical) in terms of such features as sensitivity, accuracy and precision.

1. Organochlorine compounds

The Commission considered progress in the development of multidetection systems of analysis for residues of organochlorine compounds. It agreed to appoint a working party to evaluate the advantages and disadvantages of such systems for both organochlorine and organophosphorus residues with special reference to methods for the positive identification of unknown residues, the improvement of the adsorbent Florisil, the improvement of the efficiency of acetonitrile extraction for dry goods and the improvement of selectivity by the combined use of two or more different detector systems. In doing this it would also take into account the adequacy of these systems for the measurement of organophosphorus pesticide residues in total diet studies. The use of mass spectrographic techniques for the evaluation of simpler systems of analysis was recognized; but it was considered that such methods were unlikely themselves to be widely used for routine enforcement purposes.

1.1 Evaluation

1.1.1 Multiresidue methods—by J. WILLIAM COOK, assisted by J. A. BURKE

When considering multidetection systems of residue analysis, account should be taken of versatility in relation to expense. The methods are perhaps simpler than is often thought when it is considered that up to 60 different pesticide chemicals, including a few organophosphorus compounds, can be routinely studied in a single analysis which takes only a few hours. This is more than can be accomplished by a much larger personnel team using so-called simple specific methods. It is true that the analysis must be expertly supervised, but it is unlikely that any new development in the near future will change this position. The methods available should now be critically reviewed with special reference to the compatibility of systems for organochlorine residues with those for organophosphorus residues.

The limitations of electron capture, thermionic, flame ionization and microcoulometric detectors in the gas-chromatographic analysis of pesticide residues make a close consideration of the requirements for specificity very desirable. The requirements of a specific detector are as follows:

- (i) It should achieve the same (or better) sensitivity than ECD for chlorinated pesticides; in general, 100 pg of sample injected into the gas chromatograph should be detectable;
- (ii) the sensitivity should be applicable to all types of compounds which can be analysed by gas chromatography;
- (iii) the sensitivity should also be selected in an adjustable way, so as to discriminate between the major and minor components of the sample mixture, and so as to aid peak identification.

A detector which fulfils the above requirements may prove to be too expensive to replace those now used in general pesticide residue analysis; simple detectors, such as the ECD, will continue to be used, therefore, particularly for routine and quantitative work of this kind. On the other hand, improved GC-detection systems are needed in research and development laboratories to complement the less versatile instruments generally available.

Of the alternative instrumental methods of identification at present available, only mass spectrometry (MS) provides sensitivity comparable to that of the ECD. Although aromatic compounds are detectable by MS at much lower levels than most aliphatics, the differences in MS response factors are not as great as those of the ECD. The mass spectrometer may be classified as a general detector. By using a mass spectrometer focused at a certain mass number as a GC detector while interposing slow-acting filters to reduce the noise level, 100 pg of eluant is generally detectable, and in special cases this amount may be very much less. The use of two or more mass numbers is a move in the direction of positive identification. This technique requires alternation (at 1–10 cps) between the selected mass numbers so that, unfortunately, slow-acting filters must be excluded. Sensitivity is hence reduced, but the method undoubtedly affords an elegant means of overcoming certain gas chromatographic limitations, as shown by SWEeley, ELLIOT, FRIES and RYHAGE [1]; see also SCHOMBURG and HENNEBERG [2]. In the form of “mass fragmentography” the refinement has been used by HAMMAR, HOLMSTEDT and RYHAGE [3] to determine drug metabolites in human blood. The most likely mass-spectrometric method of identifying the compound which produced a given GC peak is a recording of the entire spectrum. However, scanning mass spectrometry usually gives more information than is conveniently handled, and a correct recording of intensities requires either slow scanning or amounts of material not always available in pesticide analysis. It is possible to scan repetitively up to ten mass units at a rate of up to ten sweeps per second. Alternatively, using a mass marker the whole mass spectrum can be recorded repetitively.

It is possible that a wholly fortuitous combination of mass spectral peaks could give rise to the pattern then assumed to be the result of a certain isotope distribution. Further proof of compound identity, sufficient in fact for legal purposes, but still not absolute, may be provided if some more characteristic patterns deriving from the same compound are found in the same mass spectrum. Further proof of identity by MS in

residue analysis can be provided by making use of atomic mass defects; for this purpose a precision of the order of 0.001 mass units is required in the measurement of mass number. In fact, modern high-resolution mass spectrometers usually allow more accurate mass-number measurement than is required for the determination of the elementary composition of the ions, but need more sample than is often available in residue analysis. Accuracy just sufficient to allow calculation of elementary composition may, however, be obtained by the use of peak-matching methods at medium resolution, with concomitant smaller sample size. Although a growing need is evident, not only among residue analysts, for methods of rapid elementary analysis of fractions eluted from a gas chromatograph, neither of the above techniques can yet be readily used during the short time available as the compound emerges from the column. If mass peak positions are to be measured with sufficient accuracy at medium resolution, the Gaussian shape of the recorded traces must not be distorted. Since simple repetitive scanning very much improves the recorded shapes of mass-peaks, facilities for "instant peak-matching" are very desirable.

Data which lead to the determination of elementary composition come under the heading of positive information, but do not, of course, allow identification of a given compound. At the same time, a knowledge of the molecular formula provides the desired "platform" for further work, which begins in the library. Moreover, this approach conforms to that of "classical" organic chemistry in organizing the large amount of data which may be obtained in the future from more refined mass spectrometry linked with more sensitive versions of other identification methods such as NMR, UV or IR spectrometry.

Finally, in spite of our title, it is perhaps worthwhile to ask whether in the general sense, "positive identification" is ever possible in analytical chemistry.

2. Organophosphorus insecticide residue analysis

The Commission considered progress in collaborative studies of residues of the demeton group (*J.Assoc.Offic.Analyt.Chem.* 50, 919 (1967)) and dimethoate (*Analyst* 93, 756-766 (1968)); and reviewed the available literature on metabolites of organophosphorus insecticides in relation to the analysis of food for residues of these. There was difficulty in evaluating the importance of some of the metabolites, but it was possible to make a broad division into those insecticides for which those should be sought in analysis and those for which it was less necessary. Arrangements were made for the full publication of this review and for the continued evaluation of the progress of organophosphorus insecticide residue analysis as a whole including, specifically, the compatibility of multidetection methodology between the organochlorine and organophosphorus groups of residues.

2.1 Evaluation

2.1.1 Metabolic products—by H. FREHSE in conjunction with E. MÖLLHOFF

There is difficulty in evaluating the significance of some metabolites of organophosphorus insecticides in relation to their proportion in the total residue (derived from the same insecticide) in food. In general, however, insufficient proportions of biologically active metabolites occur in food to justify their separate estimation in analysis when studying residues arising from the use of azinphos, diazinon, dichlorvos,

fenitrothion, malathion, mevinphos, parathion, parathion-methyl and trichlorfon. Active products containing a thioether grouping (carbophenothion, demeton, demeton-methyl, disulfoton, fenthion and phorate) however, give rise to mixed residues of significance and these should be considered separately in residue analysis. The principal metabolites of phosphamidon and of dimethoate should also be separately determined.

2.1.2 *Dichlorvos residue analysis*—by K.E. ELGAR

Gas chromatography can be used for the estimation of dichlorvos residues in crops and tissues in methylene dichloride extracts without clean-up with a sensitivity of 0.05 ppm using either a chlorine or a phosphorus sensitive detector. A sensitivity of 0.01 ppm is possible with steam distillation clean-up.

3. **Organomercury fungicide residue analysis**

The Commission received reports on the progress in the development of specific residue methods for alkyl, alkoxy and aryl mercurial fungicide residues. Methyl and ethyl mercury chloride (or bromide) can be distinguished gas chromatographically with relative ease but alkoxy and phenyl mercurials were relatively less stable and gave difficulty, particularly in the extraction stage. The need for continued study in this area was stressed and arrangements were made, to keep the subject under review.

4. **Fumigant residue analysis**

The Commission reviewed progress on the development of multidetection systems for unchanged fumigant residue analysis. It was now possible to cover 19 different compounds but there was still difficulty in the case of phosphine residues. Collaborative work was deferred pending the full publication of details of the more comprehensive system and arrangements were made for the continued evaluation of progress in this field.

4.1 *Evaluation*—by W. BURNS BROWN

MALONE (4) has described conditions for the gas chromatographic separation of carbon tetrachloride, carbon disulphide, ethylene dichloride, ethylene dibromide, methyl bromide and chloroform using electron capture detection. Although there is a large difference in response in some cases, this does not prevent its successful use as a multidetection system. A study of different extraction methods for the principal fumigants had shown an acid reflux procedure was the most efficient and steam distillation the least efficient, but this work had yet to be applied to products fumigated under commercial conditions. HEUSER *et al.* [5, 6, 7] have examined extraction systems for all of these compounds and for ethylene chlorohydrin and acrylonitrile and a general procedure evolved for a wider range of compounds. The sample is shaken occasionally with acetone water 5 + 1 from a few hours (flour) up to 48 hours (grain) and a dual column separation system, each with two detectors, used. Alternative extraction with acetonitrile water 5 + 1 followed by a similar examination is useful for some resolutions. Water should be removed from the extracts before gas chromatography. Other systems for mixed residues have been described by BIELORAI and ALUMOT [8].

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IUPAC-SPONSORED MEETINGS

1969

March 17-18	Centennial Celebration of Mendeleev's Discovery of the Periodic Law (Dr G. A. TETERIN, Division of Science Teaching, UNESCO, Place de Fontenoy, Paris 7 ^e , France)	Paris (France)
April 21-25	VIth International Symposium on the Chemistry of Natural Products: Steroids and terpenes (Sociedad Química de México, Apartado postal 4-875, Ciprés 176, México 4, DF, México)	Mexico City (Mexico)
May 6-9	IIInd International Pre-Symposium on Carotenoids other than Vitamin A (Prof. O. B. WEEKS, Research Centre, New Mexico State University, Las Cruces, New Mexico 88001, USA)	Las Cruces (USA)
June 17-20	Colloque Weyl-II: The nature of metal-ammonia solutions (Prof. J. J. LAGOWSKI, Department of Chemistry, University of Texas at Austin, Austin, Texas 78712, USA)	Ithaca (USA)
June 30- July 8	XXVth International Conference of Pure and Applied Chemistry (Executive Secretary, IUPAC Secretariat, Bank Court Chambers, 2/3 Pound Way, Cowley Centre, Oxford, OX4 3YF, UK)	Cortina d'Ampezzo (Italy)
July 9-10	Symposium on the Chemical Aspects of Air Pollution (Prof. G. SARTORI, Istituto di Chimica Generale ed Inorganica, Università di Roma, Piazzale delle Scienze 5, Roma, Italy)	Cortina d'Ampezzo (Italy)
July 14-18	International Atomic Absorption Spectroscopy Conference (IAAS Conference Secretary, Society for Analytical Chemistry, 9/10 Savile Row, London W 1, UK)	Sheffield (UK)
July 14-18	International Symposium on the Chemical Control of the Human Environment (IUPAC Symposium Secretary, c/o SA Council for Scientific and Industrial Research, PO Box 395, Pretoria, Republic of South Africa)	Johannesburg (South Africa)
July 16-18	Symposium on Surface Area Determination (Dr R. H. OTTEWILL, Secretary, Symposium on Surface Area Determination, School of Chemistry, University of Bristol, Cantock's Close, Bristol BS8 1TS, UK)	Bristol (UK)
July 21-25	International Symposium on Analytical Chemistry (Mr D. M. PEAKE, Secretary, International Symposium on Analytical Chemistry, 61 Lodge Road, Walsall, Staffordshire, UK)	Birmingham (UK)
July 27- August 1	IVth International Symposium on Organometallic Chemistry (Dr E. W. ABEL, Secretary, IVth International Conference on Organometallic Chemistry, School of Chemistry, University of Bristol, Cantock's Close, Bristol BS8 1TS, UK)	Bristol (UK)
August 20-27	XXIIInd International Congress of Pure and Applied Chemistry and XIIth International Conference on Co-ordination Chemistry (Organizing Committee, XXIIInd IUPAC/XIIth ICC, Box 2249U, GPO, Melbourne, Australia 3001)	Sydney (Australia)
August 25-30	International Symposium on Macromolecular Chemistry: Kinetics and mechanism of polyreactions (Secretariat of the Symposium on Macromolecular Chemistry, Budapest II, Pusztaszeri út 59-67, Hungary)	Budapest (Hungary)
September 1-4	IVth Microsymposium: Rheology of polymer solids and concentrated solutions (Institute of Macromolecular Chemistry, Czechoslovak Academy of Sciences, Prague 6 - Petřiny, Czechoslovakia)	Prague (Czechoslovakia)
September 1-3	Vth Microsymposium: Cyclopolymers and cyclopolymerization (Institute of Macromolecular Chemistry, Czechoslovak Academy of Sciences, Prague 6 - Petřiny, Czechoslovakia)	Prague (Czechoslovakia)
September 8-11	VIth Microsymposium: Light scattering in polymer science (Institute of Macromolecular Chemistry, Czechoslovak Academy of Sciences, Prague 6 - Petřiny, Czechoslovakia)	Prague (Czechoslovakia)
September 8-12	International Symposium on Conformational Analysis (Executive Secretary, International Symposium on Conformational Analysis, 49, square Marie-Louise, Bruxelles 4, Belgium)	Brussels (Belgium)
October 16-19	International Symposium on University Chemical Education (Prof. G. ILLUMINATI, Istituto Chémico, Università di Roma, 00185 Roma, Italy)	Frascati (Italy)

1970

April 1-4	International Conference on Thermodynamics (Dr W.J. HORNIX, Secretary of Organizing Committee, Department of Applied Mathematics and Mathematical Physics, University College of South Wales, Cardiff, UK)	Cardiff (UK)
June 22-27	VIIth International Symposium on the Chemistry of Natural Products (Prof. S.N. ANANCHENKO, General Secretary, VIIth International Symposium on the Chemistry of Natural Products, Institute for Chemistry of Natural Products, Academy of Sciences of USSR, ul. Vavilova 18, Moscow 312, USSR)	Riga (USSR)
July 12-18	IIIrd International Symposium on Photochemistry (Prof. D. BRYCE-SMITH, Department of Chemistry, University of Reading, Whiteknights Park, Reading, Berkshire, UK)	St. Moritz (Switzerland)
August 25-30	International Symposium on the Chemistry of Nonbenzenoid Aromatic Compounds (Prof. S. Irô, General Secretary, International Symposium on the Chemistry of Nonbenzenoid Aromatic Compounds, Department of Chemistry, Tohoku University, Sendai, Japan)	Sendai (Japan)
September 7-11	VIth International Symposium on Microtechniques (Prof. H. MALISSA, Institut für Analytische Chemie und Mikrochemie der Technischen Hochschule Wien, Getreidemarkt 9, A-1060 Wien, Austria)	Graz (Austria)
September 11-18	XIIIth International Conference on Co-ordination Chemistry (Dr K. BUKIETŃSKA, Secretary, XIIIth International Conference on Co-ordination Chemistry, Uniwersytet Wrocławski, Katedra Chemii Nieorganicznej, Wrocław, Poland)	Zakopane/ Cracow (Poland)
September 20-24	Conference on Analytical Chemistry (Hungarian Chemical Society, Szabadság tér 17, Budapest V, Hungary)	Budapest (Hungary)
September	Symposium on Chemistry of Pesticides under Metabolic and Environmental Conditions (Prof. F. KORTE, Institute of Ecological Chemistry, Bonn University, Bonn, Germany)	Bonn (Germany)

1971

February	Symposium on Chemistry of Terminal Pesticide Residues (Dr H. HURTIG, Canada Department of Agriculture, Research Branch, Central Experimental Farm, Ottawa, Canada)	Tel Aviv (Israel)
July 19-24	XXVIth International Conference of Pure and Applied Chemistry (Executive Secretary, IUPAC Secretariat, Bank Court Chambers, 2/3 Pound Way, Cowley Centre, Oxford, OX4 3YF, UK)	Washington, DC (USA)
July 25-31	XXIIIrd International Congress of Pure and Applied Chemistry (Prof. P.D. BARTLETT, Chairman of Programme Committee, XXIIIrd International Congress of Pure and Applied Chemistry, Department of Chemistry, Harvard University, 12 Oxford Street, Cambridge, Mass. 02138, USA)	Boston (USA)
Summer	IIIrd International Conference on Crystal Growth (Dr B. MUTAF-TSHIEV, Laboratoire de Minéralogie-Cristallographie, Université d'Aix-Marseille, Marseille, France)	Marseille (France)

1972

April 3-7	International Congress on Analytical Chemistry (Prof. T. FUJINAGA, Faculty of Sciences, University of Kyoto, Kyoto, Japan)	Kyoto (Japan)
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CALENDAR OF NON-IUPAC MEETINGS

1969

March 2-7	XXth Pittsburgh Conference on Analytical Chemistry and Applied Chemistry (W. M. HICKAM, Programme Chairman, 1969 Pittsburgh Conference, Westinghouse Research Laboratories, Pittsburgh, Pa. 15235, USA)	Cleveland (USA)
March 3-6	Symposium on Protein Structure and Function (T. H. G. MICHAEL, General Manager, The Chemical Institute of Canada, 151 Slater Street, Ottawa 4, Canada)	St. Marguerite (Canada)
March 13-14	Meeting on Automation and Data Processing in Clinical Chemistry (Prof. I. TRAUTSCHOLD, Medizinische Hochschule Hannover, Klinische Biochemie, 3000 Hannover, Osterfeldstrasse 5, Germany)	Hannover (Germany)
April 13-18	157th National Meeting of The American Chemical Society (F. McLAFFERTY, Cornell University, Ithaca, N.Y. 14850, USA)	Minneapolis (USA)
April 14-18	Joint Annual Meetings of The Chemical Society (London) and The Royal Institute of Chemistry (Dr J. F. GIBSON, Conference Secretary, The Chemical Society, Burlington House, London W1V 0BN, UK)	Nottingham (UK)
April 15-16	Symposium on Industrial Crystallization (Institution of Chemical Engineers, 16 Belgrave Square, London SW1, UK)	London (UK)
April 15-18	IIIrd International Conference on Protactinium (GDCh-Geschäftsstelle, 6000 Frankfurt (M), Postfach 119075, Germany)	Schloss Elmau/ Mittenwald (Germany)
April 17-18	Symposium on Practical Rheology in Polymer Processing (Plastics Institute, 11 Hobart Place, London SW1, UK)	London (UK)
April 20-23	Vth International Conference on the Science of Ceramics (Prof. C. BROSSET, Swedish Institute for Silicate Research, Gibraltar-gatan 5, Goteborg, Sweden)	Ronneby (Sweden)
April 21-25	International Symposium on Pulp and Paper Process Control (Technical Section, Canadian Pulp and Paper Association, 2280 Sun Life Building, Montreal 2, Quebec, Canada)	Vancouver (Canada)
April 21-26	IVth Triennial Inter-American Congress of Chemical Engineering (Ing. J. SALGADO, Organizing Committee, Juez Tedin 3028, Buenos Aires, Argentina)	Buenos Aires and Montevideo (Argentina)
April 22-26	EUCHEM Conference "Metallproteide" (GDCh-Geschäftsstelle, 6000 Frankfurt (M), Postfach 119075, Germany)	Helgoland (Germany)
May 4-10	Vth EUCHEM Conference on Stereochemistry (Prof. A. KJAR, c/o Organic Chemistry Laboratory, Royal Veterinary and Agriculture College, 13 Bulowsvej, Copenhagen 5, Denmark)	Burgenstock (Switzerland)
May 8-9	IIInd International Conference on Organolead and Organozinc Chemistry (Organizing Committee, c/o Jaarbeurs, Utrecht, Netherlands)	Utrecht (Netherlands)
May 17-25	XXth Congress of The Italian Chemical Society "Giornate della Chimica 1969" (Dr L. S. SATTA, Sezione Lombarda della Società Chimica Italiana, Piazzale Rodolfo Morandi 2, 20121 Milano, Italy)	Milan (Italy)
May 19-24	International Colloquium on the Organic Chemistry of Phosphorus (P. CHABRIER, 242, bd St-Germain, Paris-7 ^e , France)	Paris (France)
May 26-30	XVth International Spectroscopy Colloquium (Dr E. ARENSI-ALVAREZ-ARENAS, General Secretary, XV Colloquium Spectroscopicum Internationale, Serrano 119, Madrid 6, Spain)	Madrid (Spain)

May 27-30	XXth Annual Meeting of Society of Physical Chemistry (Secrétaire général, Société de Chimie physique, 10, rue Vauquelin, 75 Paris-5 ^e , France)	Paris (France)
June 4-7	XXIst Congress of Union of Textile Chemists and Colorists (Rohrbacherstrasse 78, Heidelberg, Germany)	Baden-Baden (Germany)
June 16-17	Conference on Plastics (Plastics Institute, 11 Hobart Place, London SW1, UK)	London (UK)
June 16-20	IXth Conference on Carbon (Dr A.I. MEDALIA, c/o Cabot Corporation, Concord Road, Billerica, Mass. 01821, USA)	Boston (USA)
June 23- July 7	International Summer School "Chemistry of Solid/Liquid Interfaces" (Prof. B. TEZAK, Institute "Rudjer Boskovic", P.O.B. 171, Zagreb, Yugoslavia)	Herceg Novi (Yugoslavia)
July 1-3	International Symposium on Chemical Effects of Nuclear Transformations (Dr J.F. GIBSON, Scientific Affairs Officer, The Chemical Society, Burlington House, London W1V OBN, UK)	Cambridge (UK)
July 7-11	International Colloquium on Structure and Properties of Solid Surfaces (Prof. J. BÉNARD, Ecole Nationale supérieure de Chimie, 11, rue Pierre-Curie, Paris-5 ^e , France)	Paris (France)
July 7-11	IIInd International Congress of Heterocyclic Chemistry (Secrétariat du Deuxième Congrès International de Chimie hétérocyclique, Service de M. le Professeur JACQUIER, Faculté des Sciences, Place Eugène Bataillon, 34-Montpellier, France)	Montpellier (France)
July 8-10	International Symposium on Isotope Effects (Dr J.F. GIBSON, Scientific Affairs Officer, The Chemical Society, Burlington House, London W1V OBN, UK)	York (UK)
July 14-18	IVth International Congress for Pharmacology (Dr F.J. BOVE, Secretary of Organizing Committee, IVth International Congress for Pharmacology, Postfach 30, 4000 Basel 4, Switzerland)	Basle (Switzerland)
July 15-16	International Symposium on Enamine Chemistry (Dr P.W. HICKMOTT, Department of Chemistry, University of Salford, Salford M5 4WT, UK)	Salford (UK)
July 15-19	International Symposium on Nuclear Magnetic Resonance (Dr J.F. GIBSON, Scientific Affairs Officer, The Chemical Society, Burlington House, London W1V OBN, UK)	Birmingham (UK)
July 16-18	International Conference on Ion Exchange in the Process Industries (Society of Chemical Industry, 14 Belgrave Square, London SW1, UK)	London (UK)
July 22-24	International Symposium on Synthetic Methods and Rearrangements in Alicyclic Chemistry (Dr J.F. GIBSON, Scientific Affairs Officer, The Chemical Society, Burlington House, London W1V OBN, UK)	Oxford (UK)
August 11-14	International Symposium on Electron and Nuclear Magnetic Resonance (Executive Secretary, Australian Academy of Science, Gordon Street, Canberra City, ACT, Australia 2601)	Clayton (Australia)
August 12-15	IIIrd International Photoconductivity Conference (G.S. PICUS, Conference Secretary, IIIrd International Photoconductivity Conference, Hughes Research Laboratories, 3011 Malibu Canyon Road, Malibu, Calif. 90265, USA)	Palo Alto (USA)
August 13-21	VIIIth General Assembly and International Congress of International Union of Crystallography (Mrs N. FIESS, Executive Secretary, International Union of Crystallography Congress Headquarters, Room 254, ES & S, State University of New York at Stony Brook, Stony Brook, N.Y. 11790, USA)	New York (USA)

August 31– September 3	International Wood Chemistry Symposium (Profs K. V. SARKANEN and J. L. MCCARTHY, Benson Hall, University of Washington, Seattle, Washington 98105, USA)	Seattle (USA)
August 31– September 4	Ist International Conference on Calorimetry and Thermodynamics (Dr H. KEHIAIN, Secretary of Organizing Committee, Ist International Conference on Calorimetry and Thermodynamics, Institute of Physical Chemistry, Polish Academy of Sciences, PO Box 49, Warsaw 42, Poland)	Warsaw (Poland)
September 6–11	XIth Conference of International Union of Leather Chemists Societies (3 William Street, Hurstead, Rochdale, Lancashire, UK)	London (UK)
September 8–10	International Symposium on Distillation (Institution of Chemical Engineers, 16 Belgrave Square, London SW1, UK)	Brighton (UK)
September 8–13	VIIth International Congress of Clinical Chemistry (Dr M. ROTH, Secretary, VIIth International Congress of Clinical Chemistry, Palais des Expositions, 16, quai de l'Ecole de Médecine, CH-1211 Genève 4, Switzerland)	Geneva (Switzerland)
September 15–20	International Congress of Chemical Engineering, Chemical Equipment and Automation (III CHISA 1969, Czechoslovak Scientific and Technical Society, PO Box 857, Prague 1, Czechoslovakia)	Marianske Lazne (Czechoslovakia)
September 15–20	General Assembly of The German Chemical Society (GDCh-Geschäftsstelle, 6000 Frankfurt (M), Postfach 119075, Germany)	Hamburg (Germany)
September 22–27	XXth Meeting of International Committee of Electrochemical Thermodynamics and Kinetics (Dr H. TANNENBERGER, Secretary General, International Committee of Electrochemical Thermodynamics and Kinetics, c/o Institut Batelle, Centre de Recherche de Genève, 7, route de Drize, 1227 Carouge-Genève, Switzerland)	Strasbourg (France)
September 22–23	International Conference on the Use of Cyclotrons in Chemistry, Metallurgy and Biology (F. K. PYNE, Conference Secretary, International Conference on the Use of Cyclotrons in Chemistry, Metallurgy and Biology, Atomic Energy Research Establishment, Harwell, Didcot, Berkshire, UK)	Oxford (UK)
September	International Symposium on the Chemistry and Morphology of Aging (Dr D. A. BATTISTA, Chairman, Committee on Aging and Health, American Institute of Chemists, c/o FMC Corporation, PO Box 8, Princeton, N.J. 08540, USA)	Atlantic City (USA)
October 16–17	Meeting of Federation of Belgian Chemical Industries (M. J. M. DAQUETTE, Directeur, Federation of Belgian Chemical Industries, 49, square Marie-Louise, Bruxelles 4, Belgium)	Brussels (Belgium)
October	Xth European Congress on Molecular Spectroscopy: Spectroscopy of solid state (Prof. ROSEN, Institut de Physique à Sart-Tilman par Liège, Belgium)	Liège (Belgium)
December	International Colloquium on the Rare Earths (F. TROMBE, Laboratoire de Recherches sur les Terres Rares, Centre National de la Recherche Scientifique, 15, quai Anatole-France, Paris-7 ^e , France)	Paris or Grenoble (France)

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LIST OF ABBREVIATIONS

AOAC	Association of Official Agricultural Chemists
CBN	Commission on Biochemical Nomenclature
CEBJ	Commission of Editors of Biochemical Journals
CEE	Communauté Economique Européenne
CIG	Comité International de Géophysique
CIPM	Comité International de Poids et Mesures
CITCE	Comité International de Thermodynamique et Cinétique Electrochimique
CNRS	Centre national de la Recherche scientifique
COMECON	Council for Mutual Economic Assistance
COSPAR	Committee on Space Research
CSF	Compagnie Télégraphie Sans Fil
CSIRO	Commonwealth Scientific and Industrial Research Organization
DECHEMA	Deutsche Gesellschaft für chemisches Apparatewesen eV
EEC	European Economic Community
EMPA	Eidgenössische Materialprüfungs-Anstalt
EPPO	European and Mediterranean Plant Protection Organization
ETH	Eidgenössische Technische Hochschule (Zürich)
EUCEPA	European Committee on Cellulose and Paper
EUROTOX	Comité européen permanent pour la Protection des populations contre les risques de toxicité à long terme
FAGS	Fédération of Astronomical and Geophysical Services
FAO	Food and Agriculture Organization
GEFAP	Groupement européen des Associations nationales de Fabricants de Pesticides
IAEA	International Atomic Energy Agency
IAMS	International Association of Microbiological Societies
IAPT	International Association for Plant Taxonomy
IASH	International Association of Scientific Hydrology
IAU	International Astronomical Union
IBP	International Biological Programme
ICCA	International Commission for Cellulose Analysis
ICSU	International Council of Scientific Unions
ICUMSA	International Committee for the Unification of Methods of Sugar Analysis
IGU	International Geographical Union
IMU	International Mathematical Union
ISO	International Organization for Standardization
ITU	International Telecommunication Union
IUB	International Union of Biochemistry
IUBS	International Union of Biological Sciences
IUCr	International Union of Crystallography
IUGG	International Union of Geodesy and Geophysics
IUGS	International Union of Geological Sciences
IUNS	International Union of Nutritional Sciences
IUPAC	International Union of Pure and Applied Chemistry
IUPAP	International Union of Pure and Applied Physics

JCAM	Joint Commission on Atomic Masses
JCAR	Joint Commission on Applied Radioactivity
MIT	Massachusetts Institute of Technology
NAS	National Academy of Sciences
NATO	North Atlantic Treaty Organization
NBS	National Bureau of Standards
NRC	National Research Council
OECD	Organisation de Coopération et de Développement économiques
OEPP	Organisation européenne de Protection des Plantes
OMS	Organisation Mondiale de la Santé
SCAR	Scientific Committee on Antarctic Research
SCOR	Scientific Committee on Oceanic Research
UICC	Union internationale contre le Cancer
UNESCO	United Nations Educational Scientific and Cultural Organization
WHO	World Health Organization
WMO	World Meteorological Organization



**INTERNATIONAL UNION OF PURE
AND APPLIED CHEMISTRY
UNION INTERNATIONALE DE CHIMIE
PURE ET APPLIQUÉE**

**INFORMATION BULLETIN
NUMBER 35**

XXVTH CONFERENCE

30 June—8 July 1969

CORTINA (ITALY)

JUNE 1969

SECRETARY GENERAL:

Dr R. Morf, Postbox 165, CH-8058 Zürich-Airport (Switzerland)

Cable address: IUPACAIRPORT

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HQ Zürich-Airport

XXVTH IUPAC CONFERENCE

CORTINA D'AMPEZZO, ITALY, 30 JUNE—8 JULY 1969

Cortina d'Ampezzo, which the Italian National Adhering Organization has chosen for the location of the XXVth Conference, is situated in the Dolomite mountains.

Accommodation and travel

Full details of hotel accommodation and various travel schemes have already been distributed to National Adhering Organizations, Titular and Associate Members, National Representatives, and Observers. Any queries should be addressed to the IUPAC Secretariat (Bank Court Chambers, 2/3 Pound Way, Cowley Centre, Oxford OX4 3YF, England).

The nearest airports are Venice and Innsbruck. Persons proceeding to Venice will find special coaches available in Roma Square, which will take them directly to their hotels in Cortina d'Ampezzo. Anyone travelling via Innsbruck will need to continue his journey by train to Fortezza, where again coaches will be available to transport him to Cortina d'Ampezzo.

Arrangements can be made through the IUPAC Secretariat for provision of visas and for extended stays in Italy either en route to or from the Conference.

Schedule of meetings

Subject to last-minute changes, the Schedule of Meetings is as shown. Details of meeting rooms will be given to everyone on arrival at his hotel and, in addition, will be displayed on the IUPAC Notice Board in the foyer of each hotel. As far as possible, meetings will take place in the hotels at which persons are staying. The meetings of Council, Bureau and Executive Committee will be held in the Savoia Grand Hotel.

Secretariat

During the Conference the IUPAC Secretariat will be located in the Savoia Grand Hotel (Telephone: CORTINA 3201; telegraphic address: ITALCIT IUPAC CORTINA). It will be open daily from 9.00 and provide typing or photocopying facilities to assist Members and Delegates in their work.

In addition, there will be an hostess, fluent in English, in each hotel where meetings are taking place, to deal with inquiries of a general nature.

Reimbursement

For those Titular Members who have requested reimbursement of travel and subsistence at Cortina d'Ampezzo, this will be made at a Bank situated in the main street close to the Savoia Grand Hotel, between 9.00 and 12.30 and 14.30 and 16.00.

Weather and clothing

Formal dress will not be essential for any of the social functions. However, because several functions will take place out of doors, it is desirable to have available some warm clothing since the night temperature will range from 10 to 15 °C. The average daily temperature is about 25 °C.

SYMPOSIUM ON THE CHEMICAL ASPECTS OF AIR POLLUTION

Cortina d'Ampezzo (Italy), 9-10 July 1969

Under the patronage of IUPAC

Part 1: Physical and chemical transformation of pollutants in the atmosphere.

Part 2: Development of methods for the measurement of air pollutants.

Approximative number of participants: 200.

Number of papers expected: 15 short communications.

Invited lecturers (4 plenary lectures): Prof. R. TRUHAUT (University of Paris); Prof. A. LIBERTI (University of Rome); Dr S. R. CRAXFORD (Warren Spring Laboratory); Dr STEWART (Department of Health and Welfare, USA), or Prof. GEORGI (University of Frankfurt).

Summaries of the papers will be distributed to delegates at the Symposium and the final report will be published in: "Pure and Applied Chemistry."

TIME SCHEDULE OF MEETINGS FOR XXVTH IUPAC CONFERENCE

(as at 17 June 1969)

Meeting of	Monday 30 June	Tuesday 1 July	Wednesday 2 July	Thursday 3 July	Friday 4 July	Saturday 5 July	Sunday 6 July	Monday 7 July	Tuesday 8 July
Council						11-12.30 14-18		11-12.30 14-18	
Bureau					9-12 14-18				9-12 14-18
Division Presidents Executive Committee				9-12 14-18			9-12		
Interdivisional Committee on Nomenclature and Symbols					16-18				
Coordinating Committee for Analytical Methods		19-21							
Finance Committee			9-12						
Standing Committee on Congress Organization and Programmes			16-18						
Industrial Members of IUPAC					19-21				
Physical Chemistry Division									
Division Committee		9-12							
Commission I.1						9-12			
Physico-Chemical Symbols, Terminology and Units	9.30-12 14-18	9.30-12 14-18	9.30-12 14-18						
Commission I.2				9-12 14-18	9-12				
Thermodynamics and Thermochemistry			14-18	14-18					
Commission I.3			9-12	9-12 14-18	9-12				
Electrochemistry									
Commission I.4			9-12	9-12					
Data and Standards		14-18	14-18						
Commission I.5									
Molecular Structure and Spectroscopy			14-18	14-18					

	Monday 30 June	Tuesday 1 July	Wednesday 2 July	Thursday 3 July	Friday 4 July	Saturday 5 July	Sunday 6 July	Monday 7 July	Tuesday 8 July
Commission I.6 Colloid and Surface Chemistry Joint Meeting of Chairmen and Secretaries of I.3 and V.5			9-12 14-18 14-18	9-12 14-18	9-12				
Inorganic Chemistry Division									
Division Committee									
Commission II.1 Atomic Weights			9-12	14-18 9-12	18-20				
Commission II.2 Nomenclature of Inorganic Chemistry	9-12 14-18	9-12 14-18	9-12 14-18	9-12 14-18	9-12 14-18 9-12				
Commission II.3 High Temperatures and Refractories									
Organic Chemistry Division									
Division Committee									
Commission III.2 Chemical Plant Taxonomy			9-12 14-18	9-12 14-18			14-18		
Macromolecular Division									
Division Committee	10.30-12 14-19		17-20						
Analytical Chemistry Division									
Division Committee									
Commission V.1 Analytical Reactions and Reagents		9-12	9-12	14-18					

Meeting of	Monday 30 June	Tuesday 1 July	Wednesday 2 July	Thursday 3 July	Friday 4 July	Saturday 5 July	Sunday 6 July	Monday 7 July	Tuesday 8 July
Commission V.2									
Microchemical Techniques and Trace Analysis		9-12 14-18	9-12 14-18						
Commission V.3					9-12				
Analytical Nomenclature		14-18	14-18						
Commission V.4									
Spectrochemical and other Optical Procedures for Analyses	16-18	9-12 14-18	9-12 14-18						
Commission V.5		9-12	9-12		9-12				
Electroanalytical Chemistry		14-18							
Commission V.6			9-12						
Equilibrium Data			14-18						
Commission V.7									
Analytical Radiochemistry and Nuclear Materials		9-12 14-18	9-12 14-18						
Liaison Meeting on Separation Processes (V.3, V.6)									
Joint Meeting of V.1 and VI.1		16-18				9.30-10.30			
Joint Meeting of Chairmen and Secretaries of I.3 and V.5									
Open Meeting of Analytical Chemistry Division			14-18	9-12	14-18				
Applied Chemistry Division									
Division Committee	14-18								
Section VI.1			9-10	18-20 10-12					
Food					14-16 9-12				
Commission VI.1.1			10-12	9-10					
Trace Substances			14-18						
Commission VI.1.2			10-12	9-10	9-12				
Food Additives			14-18						
Section VI.2		9-12	9-12						
Fermentation Industries		14-18	14-18						

Meeting of	Monday 30 June	Tuesday 1 July	Wednesday 2 July	Thursday 3 July	Friday 4 July	Saturday 5 July	Sunday 6 July	Monday 7 July	Tuesday 8 July
Section VI.3			9-12						
Oils and Fats			14-18						
Section VI.4		9-12	9-12						
Toxicology and Industrial Hygiene		14-18							
Section VI.5		9-12					9-12		
Pesticides									
Commission VI.5.1			9-12						
Terminal Pesticide Residues		14-18	14-18			14-18			
Commission VI.5.2				9-12	9-12	9-12			
Pesticide Residue Analysis					14-18				
Section VI.6		9-12	9-12						
Organic Coatings		14-18	14-18						
Section VI.8			9-12						
Water, Sewage, and Industrial Wastes			14-18						
Joint Meeting of V.1 and VI.1		16-18				9.30-10.30			
Open Meeting of Applied Chemistry Division				14-18					

Clinical Chemistry Section

Commission on Teaching

9-12
14-18

Social Functions

A full social programme has been arranged by our hosts in Cortina for all Conference participants and their families as follows:

Ice-hockey Match at the Olympic Stadium	Wednesday, 2 July
Reception by Aziende Autonome Soggiorno e Turismo	Thursday, 3 July
Reception by the Municipality of Cortina d'Ampezzo	Saturday, 5 July
Reception by the Italian Research Council	Sunday, 6 July

In addition there will be a full-day and a half-day excursion in the Dolomites for wives and families of Conference participants.

ORDRE DU JOUR DES RÉUNIONS DU CONSEIL A LA XXV^E CONFÉRENCE DE IUPAC

Cortina d'Ampezzo, le 5 et le 7 juillet 1969

- 1 Ordre du jour définitif
- 2 Approbation du Procès verbal
- 3 Annonce des candidatures aux élections
- 4 Date des élections
- 5 Rapport statutaire du Président sur l'état de l'Union
- 6 Rapport biennal du Trésorier
- 7 Rapport du Comité financier
- 8 Organisations adhérentes, changement de catégorie pour le Brésil, le Japon et la Roumanie
- 9 Budget pour 1970 et projet de budget pour 1971
- 10 Structure des contributions
- 11 Détermination des contributions annuelles pour 1970 et 1971
- 12 Rapport du Comité pour l'enseignement de la Chimie
- 13 Rapport sur les publications
- 14 Rapport des Présidents de Divisions et de la Section de Chimie clinique
- 15 Adoption des règles de nomenclature définitives
- 16 Propositions du Bureau pour de nouvelles unités
- 17 Approbation des décisions prises par le Bureau et le Comité exécutif
- 18 Elections
- 19 Date et lieu de la Conférence et du Congrès en 1973
- 20 Divers

AGENDA FOR THE XXVTH IUPAC CONFERENCE COUNCIL MEETINGS

Cortina d'Ampezzo — 5 and 7 July 1969

- 1 Definitive Agenda
- 2 Approval of Minutes
- 3 Announcement of Nominations of Candidates for Elections
- 4 Announcement of Time of Elections
- 5 Statutory Report of the President on the State of the Union
- 6 Biennial Report of the Treasurer
- 7 Report of the Finance Committee
- 8 Adhering Organizations: Change of category for Brazil, Japan and Rumania
- 9 Budget for 1970 and Budget Estimate for 1971
- 10 Dues Structure
- 11 Fixing the Annual Dues for 1970 and 1971
- 12 Report of the Committee on Teaching of Chemistry
- 13 Report on Publications
- 14 Reports of the Division Presidents and the Clinical Chemistry Section
- 15 Adoption of Final Nomenclature Rules
- 16 Bureau Proposals for New Units
- 17 Ratification of Decisions taken by Bureau and Executive Committee
- 18 Elections
- 19 Date and Place of Conference and Congress in 1973
- 20 Any other business

LETTER OF THE SECRETARY GENERAL CONCERNING THE CANDIDATES

750/RM/LW

Zürich, le 8 mai 1969

Le Secrétaire général
aux Organisations adhérentes et aux
Membres du Bureau

Objet:

XXV^e Conférence, point 3 de l'ordre du
jour

*Informations statutaires en ce qui concerne
les candidatures proposées*

Chers Collègues,

Des renseignements préliminaires vous
ont été transmis par mes lettres du 4 août
et 14 décembre 1968 au sujet des propo-
sitions faites pour les candidatures des
membres élus du Bureau.

Les propositions reçues ici, en bonne
et due forme et à la date prévue, sont les
suivantes:

Pour le poste de vice-président (celui-ci
assumera en 1971 automatiquement la
présidence):

Prof. J. BÉNARD (Paris)

Le Prof. BÉNARD a été proposé non seule-
ment par l'Organisation adhérente fran-
çaise, mais déjà antérieurement par le
Comité national français et par diffé-
rentes autres organisations ou personnes
parmi lesquelles je désire mentionner:

Deutscher Zentralausschuss für Chemie, Frankfurt (Main)
The Division of Chemistry and Chemical Technology, Washington
The British National Committee for Chemistry, London

Veuillez trouver ci-inclus une biographie
et une copie de mon accusé de réception
officiel.

750/RM/LW

Zürich, 8 May 1969

The Secretary General
to Adhering Organizations
and Bureau Members

Re:

Item 3 of the Agenda for the
XXVth IUPAC Conference
*Statutory Information as to the Candidates
who have been proposed*

Dear Colleagues,

Preliminary information regarding the
nomination of candidates for the Bureau
positions has been sent to you by my
letters dated 4 August and 14 December
1968.

The following nominations for candi-
dates have been duly received in good
time:

For the post of Vice-President who in
1971 will automatically assume the office
of President:

Prof. BÉNARD has been proposed not only
by the French National Adhering Orga-
nization, but already before by the French
National Committee and by various other
organizations or persons, among whom
I only mention here:

A biography and a copy of my official
acknowledgment are appended.

Election des membres élus du Bureau

Election of the Elected Members to the Bureau

Jusqu'au 7 mai 1969 (date-limite statutaire) ont été reçues les propositions des candidats suivants en qualité de membres élus du Bureau:

Up to 7 May 1969 (the statutory deadline) the following nominations for candidates for elected members to the Bureau were duly received:

Prof. TONG HYUK AHN (Seoul, Republic of Korea)

Mr. PHILIP M. ARNOLD (Bartlesville, USA)

Prof. L. H. BRIGGS (Auckland, New Zealand)

Prof. M. CAIS (Haifa, Israel)

Prof. E. A. M. FERNAND DAHMEN (Enschede, Netherlands)

Dr PIERRE R. GENDRON (Pointe Claire, Canada)

Prof. Dr Ing. VLASTIMIL HEROUT (Prague, Czechoslovakia)

Prof. H. MALISSA (Vienna, Austria),

proposé pour réélection pour 4 années

proposed for re-election for a second term of 4 years

Prof. S. RANGASWAMI (Delhi, India)

Prof. Dr GÉZA SCHAY (Budapest, Hungary)

Prof. GEORGES SMETS (Louvain, Belgium)

Prof. HEIKKI SUOMALAINEN (Helsinki, Finland)

Prof. F. L. WARREN (Rondebosch, Cape, South Africa)

Dr WILLIAM ZATTAR (Rio de Janeiro, Brazil)

Dans sa lettre du 6 mars 1969, M. le Prof. L. MARION, quoique proposé pour réélection comme membre du Bureau pour quatre années, m'a informé qu'il ne désire pas se présenter à une réélection: voir ma lettre du 31 mars 1969.

En dernier lieu et afin de vous donner une image complète, je répète ici les noms des membres du Bureau qui continueront leur mandat jusqu'en 1971, à savoir:

In his letter of 6 March 1969 Prof. L. MARION, although proposed for re-election as a member of the Bureau for another term of four years, has notified me that he does not wish to stand for re-election (see my letter of 31 March 1969).

Finally, in order to give you a full picture, I repeat here the names of those elected members who will serve another two years:

Prof. G. SARTORI (Italy)

Prof. S. SHIBATA (Japan)

Prof. F. WEYGAND (Germany)

Prof. J. LECOMTE (France)

Sir HAROLD THOMPSON (United Kingdom)

Les présidents de Divisions qui sont membres ex-officio du Bureau seront les suivants:

Also the Division Presidents who are ex-officio Bureau Members will be as follows:

Dr GUY WADDINGTON (USA) (Division I)

Prof. J. BÉNARD (France) (Division II)

Prof. D. H. R. BARTON (UK) (Division III)

Prof. O. WICHTERLE (Czechoslovakia) (Division IV)

Prof. W. KEMULA (Poland) (Division V)

Dr W. GALLAY (Canada) (Division VI)

Conformément aux Statuts 2.222, le scrutin pour l'élection de membres élus doit être conduit selon une procédure à déterminer par le Bureau pour chaque assemblée du Conseil.

Conformément aux Statuts, les Organisations adhérentes de la catégorie D ont droit à 1 voix, celles de la catégorie C à 2, des catégories B1 et B2 à 4, et A1, A2, A3, etc. à 6 voix. Les bulletins de vote seront distribués à Cortina d'Ampezzo au chef de la délégation officielle de chaque délégation nationale.

Une courte biographie de chaque candidat sera envoyée séparément.

Un dossier comprenant la documentation complète sera remis à chaque délégué lors de son inscription à Cortina au Savoia Grand Hôtel.

Pour des raisons d'économie, un jeu seulement de la documentation complète sera envoyé aux Organisations adhérentes. Toutefois, si celles-ci en désiraient davantage, le Secrétariat général se ferait un plaisir de la leur envoyer sur demande.

Veuillez agréer, chers Collègues, l'assurance de mes sentiments distingués.

Secretary General
Dr RUDOLF MORF

"For the election of Elected Members the ballot shall be conducted in accordance with a procedure to be determined by the Bureau for each Council meeting." (By-law 2.222 of the Statutes.)

According to the Statutes, Adhering Organizations of category D have 1 vote, category C 2 votes, categories B1 and B2 4 votes and categories A1, A2, A3, etc. 6 votes. Ballot papers will be distributed in Cortina d'Ampezzo to the leader of the official delegation of each National Adhering Organization.

Short biographies of all candidates will be sent separately.

A full and complete file containing all pertinent documents will be handed over to each delegate at his registration at the Savoia Grand Hotel in Cortina.

For reasons of economy we are sending only one preliminary set of documents to each National Adhering Organization. However, if more copies are required, we would be very pleased to send them.

**OFFICIAL DELEGATES OF NATIONAL ADHERING
ORGANIZATIONS AT THE XXVTH CONFERENCE**

**DÉLÉGUÉS OFFICIELS DES ORGANISATIONS NATIONALES
ADHÉRENTES AUPRÈS DE LA XXV^e CONFÉRENCE**

as at 17 June 1969

(Unless he is also an Official Delegate from a National Adhering Organization, a Bureau Member is entitled to vote only on scientific matters. An Observer or Secretary to a Delegation is not entitled to vote on any matter.)

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Dr D.D. PERRIN, Department of Medical Chemistry, John Curtin School of Medical Research, Australian National University, Canberra, A.C.T. 2600

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XIth INTERNATIONAL CONFERENCE ON COORDINATION CHEMISTRY

Haifa and Jerusalem, 8-18 September 1968

The Conference was organized by the Israel Chemical Society and sponsored by the International Union of Pure and Applied Chemistry. The Opening Ceremony was held in the Winston Churchill Auditorium on the campus of the Technion—Israel Institute of Technology, Haifa. Prof. D. GINSBURG, President of the Conference, chaired the evening's proceedings and gave the welcoming address.

The Scientific Program began with a Plenary Symposium on "Coordination compounds in homogeneous catalysis", the main symposium lecture being presented by Prof. J. HALPERN (USA). This was followed by four shorter lectures and a one-hour general discussion in which the five speakers answered questions and comments contributed by the audience.

Additional Plenary Symposia, with the same format as described above, were held as follows:

- "Photochemistry in coordination compounds"—main lecture by Prof. A. W. ADAMSON (USA)
- "Kinetics and mechanism of reactions of coordination compounds"—main lecture by Prof. M. EIGEN (Germany)
- "Coordination compounds in non-aqueous solvents"—main lecture by D. L. I. KATZIN (USA)
- "Coordination compounds in solvent extraction"—main lecture by Prof. H. FREISER (USA)

In addition to the Plenary Symposia, the program included three Plenary Lectures:

- "The role of transition metals in the chemical synthesis of corrins" by Prof. A. ESCHENMOSER (Switzerland)
- "A survey of recent X-ray structural studies of organometallic compounds" by Mr O.S. MILLS (UK)
- "Mass-action law versus non-ideal behavior in distribution equilibrium" by Prof. Y. MARCUS (Israel)

and there were four parallel sessions held in Haifa and two parallel sessions in Jerusalem. A total of 156 papers (112 in Haifa and 44 in Jerusalem) were presented in these sessions.

The eight Plenary and Symposia Main Lectures are to be printed in the IUPAC journal, *Pure and Applied Chemistry*, and published as a specially bound reprint from Butterworths, London. Long abstracts of papers contributed to the XIth ICCS were printed by the photographic reproduction method and published as a bound volume entitled "Progress in Coordination Chemistry", Proceedings of the XIth ICCS. The publishing firm Elsevier (Amsterdam) have undertaken the world-wide distribution of this book.

The Social Program included receptions by the Presidents of the Technion and the Hebrew University and by the Mayors of Haifa and Jerusalem. All foreign participants were invited to spend an evening as guests in Israeli homes. There was also a beach outing which included swimming in the Mediterranean, a picnic meal and a visit to the Caesarea excavations, following which the Israel Chamber Orchestra gave a special

concert in the Roman Amphitheatre in Caesarea. One of the non-chemical but nevertheless scientific highlights of the Conference was the lecture by Prof. YIGAL YADIN on "Masada", at the Hebrew University Wise Auditorium in Jerusalem.

The Conference was attended by 635 participants (including accompanying persons) from the following 29 countries: Austria, Australia, Belgium, Brazil, Canada, Czechoslovakia, Denmark, Ethiopia, France, Finland, Germany, Hong Kong, India, Israel, Italy, Japan, Korea, Netherlands, New Zealand, Norway, Portugal, Rumania, Spain, Sweden, Switzerland, Turkey, United Kingdom, United States, Yugoslavia.

MICHAEL CAIS, Chairman, XIth ICC

TENTATIVE

NOMENCLATURE RULES

5. ISO- AND HETEROPOLYANIONS

5.1 Isopolyanions

5.11 Without recourse to structural information, salts containing polyanions may be given their complete stoichiometric name, according to Rule 2.24.

Examples

- | | |
|---|--|
| 1. $\text{Na}_2\text{S}_2\text{O}_7$ | disodium heptaoxodisulfate |
| 2. $\text{Na}_2\text{S}_2\text{O}_5$ | disodium pentaoxodisulfate |
| 3. $\text{K}_2\text{H}_2\text{P}_2\text{O}_6$ | dipotassium dihydrogen hexaoxo-diphosphate |
| 4. $\text{Na}_2\text{Mo}_6\text{O}_{18}$ | disodium octadeca oxohexamolybdate |

5.12 Anions of polyacids derived by condensation of molecules of the same monoacid, containing the characteristic element in the oxidation state corresponding to its Group number, are named by indicating with Greek numerical prefixes the number of atoms of that element. It is not necessary to give the number of oxygen atoms when the charge of the anion or the number of cations is indicated.

Examples

- | | |
|--|---|
| 1. $\text{S}_2\text{O}_7^{2-}$ | disulfate(2-) |
| 2. $\text{Si}_2\text{O}_7^{6-}$ | disilicate(6-) |
| 3. $\text{Te}_4\text{O}_{14}^{4-}$ | tetratellurate(4-) |
| 4. $\text{Cr}_4\text{O}_{13}^{2-}$ | tetrachromate(2-) |
| 5. $\text{P}_3\text{O}_{10}^{5-}$ | triphosphate(5-) |
| 6. $\text{Mo}_7\text{O}_{24}^{6-}$ | heptamolybdate(6-) |
| 7. $\text{Na}_2\text{B}_4\text{O}_7$ | disodium tetraborate |
| 8. NaB_5O_8 | sodium pentaborate |
| 9. $\text{Ca}_3\text{Mo}_7\text{O}_{24}$ | tricalcium heptamolybdate |
| 10. $\text{Na}_7\text{HNb}_5\text{O}_{19} \cdot 15\text{H}_2\text{O}$ | monohydrogen heptasodium hexaniobate-15-water |
| 11. $\text{K}_2\text{Mg}_2\text{V}_{10}\text{O}_{28} \cdot 16\text{H}_2\text{O}$ | dimagnesium dipotassium decavanadate-16-water |

Note

Trivial prefixes, *e.g.* para and meta, have been used to distinguish different anions with the same number of atoms of the characteristic element (para- and meta-dodecalwolframate).

♦ Comments to these Rules should be sent to Prof. K.A. JENSEN, Kemisk Lab. II, H.C. Ørsted Inst., Universitetsparken 5, Copenhagen Ø (Denmark).

5.13 When the characteristic element is partially or wholly present in a lower oxidation state than corresponds to its Group number, its oxidation state(s) may be indicated by Stock number(s). If evidence is available, more than one Stock number may be used.

Examples

- | | |
|--|---|
| 1. $[\text{S}_2\text{O}_5]^{2-}$ | disulfate(IV)(2-) |
| 2. $[\text{H}_2\text{P}_2\text{O}_5]^{2-}$ | dihydrogendiphosphate(III)(2-)
(trivial name diphosphite) |
| 3. $[\text{HO}_2\text{P}-\text{O}-\text{PO}_3\text{H}]^{2-}$ | dihydrogendiphosphate(III, V)(2-) |
| 4. $[\text{HO}_3\text{P}-\text{PO}_3\text{H}]^{2-}$ | dihydrogendiphosphate(IV)(2-)
(trivial name hypophosphate) |
| 5. $[\text{Mo(V)}_2\text{Mo(VI)}_4\text{O}_{18}]^{2-}$ | hexamolybdate(2V, 4VI)(2-) |

5.14 Cyclic and straight chain structures may be distinguished by means of the prefixes *cyclo-* and *catena-*, although the latter may usually be omitted.

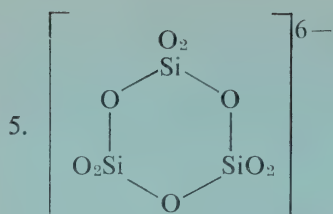
Examples

- | | |
|---|------------------------------|
| 1. $\left[\begin{array}{ccc} \text{O} & \text{O} & \text{O} \\ \text{OP}-\text{O}-\text{P}-\text{O}-\text{PO} \\ \text{O} & \text{O} & \text{O} \end{array} \right]^{5-}$ | triphosphate |
| 2. $\left[\begin{array}{c} \text{O}_2 \\ \text{P} \\ \text{O} \quad \text{O} \\ \text{O}_2\text{P} \quad \text{PO}_2 \\ \text{O} \end{array} \right]^{3-}$ | <i>cyclo</i> -triphosphate |
| 3. $[\text{O}(\text{PO}_3)_n]^{(n+2)-}$ | <i>catena</i> -polyphosphate |
| 4. $\left[\begin{array}{ccc} \text{O} & \text{O} & \text{O} \\ \text{OSi}-\text{O}-\text{Si}-\text{O}-\text{SiO} \\ \text{O} & \text{O} & \text{O} \end{array} \right]^{8-}$ | trisilicate |

Examples

- | | |
|--|---|
| $(\text{BaSiO}_3)_x$ | barium <i>ino</i> -polymetasilicate |
| $(\text{Ca}_3\text{Si}_4\text{O}_{11})_x$ | tricalcium <i>ino</i> -polytetrasilicate |
| $(\text{Na}_2\text{Si}_2\text{O}_5)_x$ | disodium <i>phyllo</i> -polydisilicate |
| $[\text{Mg}_3(\text{OH})_2\text{Si}_4\text{O}_{10}]_x$ | trimagnesium dihydroxide <i>phyllo</i> -polytetrasilicate |

♦ In mineralogy and geochemistry silicates containing chains (single or double), sheets or three-dimensional frameworks are designated by the prefixes *ino-*, *phyllo-* or *tecto-*, respectively.



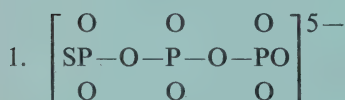
cyclo-trisilicate



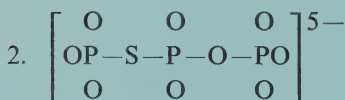
tetrapotassium tetrahydrogen
cyclo-tetrasilicate

5.15 Thioacids, peroxyacids, amidoacids, etc., derived from isopolyacids are named by adding the prefixes thio-, peroxy-, amido-, etc. to the name of the parent acid. If there is a possibility of isomerism, and the structure of the compound is known, the atom or atoms of the characteristic element, to which the group substituting oxygen is bonded, is indicated by numbers. For this purpose the atoms of the characteristic elements are numbered consecutively along the chain. The direction of numbering is chosen to give substituting atoms lowest possible locants; the element occurring lower takes precedence.

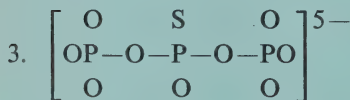
Examples



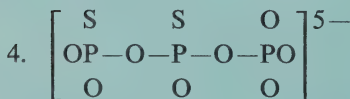
1-thiotriphosphate(5-)



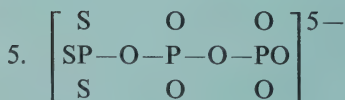
(1,2- μ)-thio-triphosphate(5-)



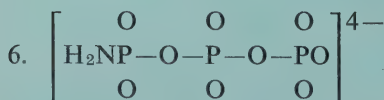
2-thiotriphosphate(5-)



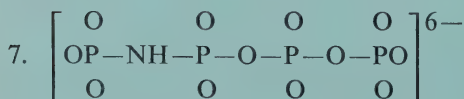
1,2-dithiotriphosphate(5-)



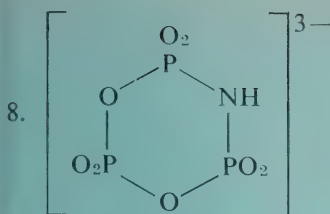
1,1,1-trithiophosphate(5-)



1-amidotriphosphate(4-)



(1,2- μ)-imido-tetraphosphate(6-)



cyclo-μ-imido-triphosphate

Note

If most of the oxygen atoms of the oxo acid have been substituted, the oxygen atoms should be indicated and the name formed according to the rules of Section 7.

Examples

- | | |
|---|---|
| 1. $[\text{F}_5\text{As}-\text{O}-\text{AsF}_5]^{2-}$ | <i>μ-oxo-decafluorodiarсенate(2-)</i> |
| 2. $[(\text{O}_2)_2\text{OCr}-\text{O}-\text{O}-\text{CrO}(\text{O}_2)_2]^{2-}$ | <i>μ-peroxo-1,2-dioxo-1,1,2,2-tetraperoxodichromate(2-)</i> |
| 3. $[\text{S}_3\text{P}-\text{O}-\text{PS}_2-\text{O}-\text{PS}_3]^{5-}$ | <i>di-μ-oxo-octathiotriphosphate(5-)</i> |

5.16 Polyanions containing two or more atoms of the characteristic element bonded together are generally named according to Rule 5.3.

5.2 Heteropolyanions

5.21 Heteropolyanions with a chain or ring structure

5.211 Dinuclear anions are named by treating the anion which comes first in alphabetical order as the ligand on the characteristic atom of the second.

Examples

- | | |
|---|------------------------------|
| 1. $[\text{O}_3\text{P}-\text{O}-\text{SO}_3]^{3-}$ | <i>phosphatosulfate(3-)</i> |
| 2. $[\text{O}_3\text{S}-\text{O}-\text{CrO}_3]^{2-}$ | <i>chromatosulfate(2-)</i> |
| 3. $[\text{O}_3\text{Se}-\text{O}-\text{SO}_3]^{2-}$ | <i>selenatosulfate(2-)</i> |
| 4. $[\text{O}_3\text{Cr}-\text{O}-\text{SeO}_3]^{2-}$ | <i>chromatoselenate(2-)</i> |
| 5. $[\text{O}_3\text{As}-\text{O}-\text{PO}_3]^{4-}$ | <i>arsenatophosphate(4-)</i> |

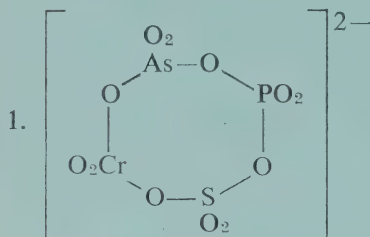
5.212 Longer chains are named similarly (unless the chain contains an obvious central atom, in which case Rule 5.214 applies), beginning with the end group which comes first in alphabetical order and treating the chain with $(n-1)$ units as the ligand on the other end group.

Examples

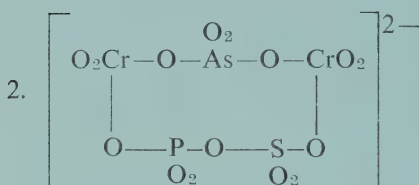
- | | |
|---|--|
| 1. $[\text{O}_3\text{Cr}-\text{O}-\text{AsO}_2-\text{O}-\text{PO}_3]^{4-}$ | <i>(chromatoarsenato)phosphate(4-)</i> |
| 2. $[\text{O}_3\text{Cr}-\text{O}-\text{PO}_2-\text{O}-\text{AsO}_3]^{4-}$ | <i>(arsenatophosphato)chromate(4-)</i> |
| 3. $[\text{O}_3\text{As}-\text{O}-\text{AsO}_2-\text{O}-\text{PO}_3]^{5-}$ | <i>(diarsenato)phosphate(5-)</i> |
| 4. $[\text{O}_3\text{S}-\text{O}-\text{CrO}_2-\text{O}-\text{AsO}_2-\text{O}-\text{PO}_3]^{4-}$ | <i>{(phosphatoarsenato)chromato}-sulfate(4-)</i> |

5.213 Cyclic heteropolyanions are named in a manner similar to those with a chain structure, the starting point and direction of citation of the units being chosen according to alphabetical priority.

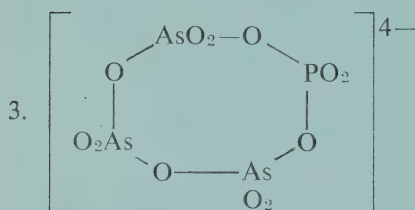
Examples



cyclo-arsenatochromatosulfato-phosphate(2-)



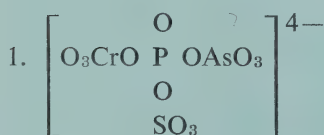
cyclo-(arsenatochromato)phosphato-sulfatochromate(2-)



cyclo-(triarsenato)phosphate(4-)

5.214 In polyanions with an obvious central atom the peripheral anions are named as ligands on the central atom and cited in alphabetical order.

Examples



arsenatochromatosulfatophosphate (4-)



trismolybdatoarsenate(3-)



bisarsenatophosphate(5-)



bisphosphatoarsenate(5-)

Note

When the central atom has no oxo ligand this name is identical with that obtained by applying the nomenclature of coordination chemistry, *e.g.* $[\text{B}(\text{ONO}_2)_4]^-$, tetranitratoborate.

5.22 *Condensed heteropolyanions*

The three-dimensional frameworks of linked WO_6 , MoO_6 , etc., octahedra surrounding the central atom are designated by the prefixes wolframo, molybdo, etc., *e.g.*

wolframophosphate (tungstophosphate), *not* phosphowolframate (phosphotungstate). The numbers of atoms of the characteristic element are indicated by Greek prefixes or numerals.

If the oxidation number has to be given, it may be necessary to place it immediately after the atom referred to and not after the ending -ate, in order to avoid ambiguity.

Examples

- | | |
|---|--|
| 1. $[\text{PW}_{12}\text{O}_{40}]^{3-}$ | dodecawolframophosphate(3-) or
12-wolframophosphate(3-) |
| 2. $[\text{PV}_2\text{Mo}_{10}\text{O}_{39}]^{3-}$ | decamolybdodivanadophosphate(3-) |
| 3. $[\text{Co}^{\text{II}}\text{Co}^{\text{III}}\text{W}_{12}\text{O}_{42}]^{7-}$ | dodecawolframocobalt(II)cobalt
(III)ate |
| 4. $[\text{Mn}^{\text{IV}}\text{Mo}_9\text{O}_{32}]^{6-}$ | enneamolybdomanganate(6-) |
| 5. $[\text{Ni}(\text{OH})_6\text{W}_6\text{O}_{18}]^{4-}$ | hexahydroxohexawolframo-
niccolate(4-) |
| 6. $[\text{IW}_6\text{O}_{24}]^{5-}$ | hexawolframoperiodate(5-) |
| 7. $[\text{CeMo}_{12}\text{O}_{42}]^{8-}$ | dodecamolybdocerate(IV)(8-) |
| 8. $[\text{Cr}^{\text{III}}\text{Mo}_6\text{O}_{21}]^{3-}$ | hexamolybdochromate(III)(3-) |
| 9. $[\text{P}(\text{V})_2\text{Mo}_{18}\text{O}_{62}]^{6-}$ | 18-molybdodiphosphate(V)(6-) |
| 10. $[\text{P}(\text{III})_2\text{Mo}_{12}\text{O}_{41}]^{4-}$ | dodecamolybdodiphosphate(III)(4-) |
| 11. $[\text{S}(\text{IV})_2\text{Mo}_5\text{O}_{21}]^{4-}$ | pentamolybdodisulfate(IV)(4-) |

The names of salts and free acids are given in the usual way, *e.g.*:

- | | |
|--|---|
| $[\text{NH}_4]_6[\text{TeMo}_6\text{O}_{24}] \cdot 7\text{H}_2\text{O}$ | hexaammonium hexamolybdo-
tellurate heptahydrate |
| $\text{Li}_3\text{H}[\text{SiW}_{12}\text{O}_{40}] \cdot 24\text{H}_2\text{O}$ | trilithium hydrogen dodecawolframo-
silicate-24-water |
| $\text{H}_4[\text{SiW}_{12}\text{O}_{40}]$ | tetrahydrogen dodecawolframo-
silicate or dodecawolframosilicic acid |

5.3 A general nomenclature for polyanions with ring or chain structure

A rational system for naming polyanions with ring or chain structure may be based upon the names of the parent—real or hypothetical—hydrides. Detailed rules for the naming of the latter compounds will be given in Nomenclature of Organic Chemistry Section D, but the following examples will suffice here to illustrate how the names of the parent hydrides are formed, a) when the structure contains several different atoms, b) when the structure contains two kinds of atoms in alternating positions, and c) when all atoms of the chain or ring are identical:

- | | |
|--|---|
| a) $\text{H}_2\text{P}-\text{NH}-\text{PH}-\text{S}-\text{PH}_2$ | 2-thia-4-aza-1,3,5-triphospha-
pentahetrane \diamond |
| b) $\text{H}_2\text{P}-\text{O}-\text{PH}-\text{O}-\text{PH}_2$ | triphosphoxane |
| c) $\text{H}_2\text{P}-\text{PH}-\text{PH}_2$ | triphosphane |

\diamond The chain is numbered from the end which leads to a lower locant at the first possible point of difference in the locants for the “a” terms as cited in the Table, and the “a” terms are arranged in this order.

Polyanions may be derived from these hydrides by depriving them of all hydrogen atoms in the form of hydride ions; to the cation thus formed, oxide ions, sulfide ions and various other anions or possibly free atoms (with the increase of the valences of chain or ring atoms) are added to form the final anion, which is designated by the suffix -ate. Thus, *e.g.* the name diphosphanate indicates an anion with a P—P core, whether both phosphorus atoms are trivalent, one is trivalent and the other pentavalent, or both are pentavalent.

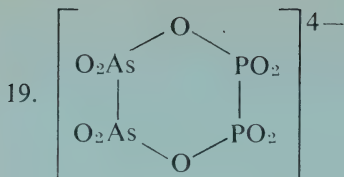
As is seen from some of the following examples this nomenclature leads to complicated—or at least unfamiliar—names for many simple anions which can satisfactorily be named by Rules 5.11, 5.16 and 5.21. However, it makes it possible to name very complex structures, with several different atoms or with the same element in different oxidation states.

5.31 The name of the anion is derived from the name of the chain or ring by naming all atoms (including hydrogen, indicated by hydrido) and radicals attached to the chain or ring as anionic ligands (Rule 7.3) and completing the name by adding the suffix -ate. The charge of the resulting anion is indicated, if necessary, with the Ewens-Bassett number. It is not necessary to indicate the valency state of the various elements because the structure follows unambiguously when the number and names of all ligands and the charge of the anion (the Ewens-Bassett number) or the number of cations are given. The ligands are cited in alphabetical order.

Examples

1. $\left[\begin{array}{cc} \text{O} & \text{O} \\ \text{HP} & \text{—PH} \\ \text{O} & \text{O} \end{array} \right]^{2-}$ 1,2-dihydridotetraoxodiphosphanate(2-)
2. $\left[\begin{array}{cc} \text{O} & \text{O} \\ \text{HP} & \text{—PO} \\ \text{O} & \text{O} \end{array} \right]^{3-}$ hydridopentaoxodiphosphanate(3-)
3. $\left[\begin{array}{cc} \text{O} & \text{O} \\ \text{OP} & \text{—PO} \\ \text{O} & \text{O} \end{array} \right]^{4-}$ hexaoxodiphosphanate(4-)
4. $\left[\begin{array}{ccc} \text{O} & \text{H} & \text{O} \\ \text{HP} & \text{—P—} & \text{PH} \\ \text{O} & \text{O} & \text{O} \end{array} \right]^{2-}$ 1,2,3-trihydridopentaoxotriphosphanate(2-)
5. $\left[\begin{array}{cccc} \text{O} & \text{O} & \text{O} & \text{O} \\ \text{OP} & \text{—O—P—O—P—O—PO} \\ \text{O} & \text{O} & \text{O} & \text{O} \end{array} \right]^{6-}$ decaoxotetraphosphoxanate(6-)
(= tetraphosphate)
6. $\left[\begin{array}{ccc} \text{O} & \text{O} & \text{O} \\ \text{HP} & \text{—O—P—O—PH} \\ \text{O} & \text{O} & \text{O} \end{array} \right]^{3-}$ 1,5-dihydrido-hexaoxophosphoxanate(3-)
7. $\left[\begin{array}{cc} \text{O} & \text{O} \\ \text{HP} & \text{—O—PS} \\ \text{O} & \text{S} \end{array} \right]^{3-}$ 1-hydrido-3,3-dithio-1,1,3-trioxodiphosphoxanate(3-)

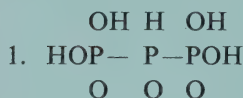
8. $\left[\begin{array}{ccc} \text{O} & \text{O} & \text{O} \\ \text{ClP}-\text{O}-\text{P}-\text{PNH}_2 \\ \text{H} & \text{O} & \text{O} \end{array} \right]^{2-}$ 4-amino-1-chloro-1-hydrido-1,3,3,4,4-pentaoxo-2-oxa-1,3,4-triphosphatetrahtranate(2-)
9. $\left[\begin{array}{ccc} \text{O} & \text{O} & \text{O} & \text{O} \\ \text{OP}-\text{P}-\text{O}-\text{P}-\text{PO} \\ \text{O} & \text{O} & \text{O} & \text{O} \end{array} \right]^{6-}$ decaoxo-3-oxa-1,2,4,5-tetraphosphapentahetranate(6-)
or (2- μ)-oxo-bis(pentaoxodiphosphanate)(6-)
10. $\left[\begin{array}{ccccccc} \text{O} & \text{O} & \text{O} & \text{O} & \text{O} & \text{O} & \text{O} \\ \text{OP}-\text{O}-\text{P}-\text{P}-\text{O}-\text{P}-\text{O}-\text{P}-\text{PO} \\ \text{O} & \text{O} & \text{O} & \text{O} & \text{O} & \text{O} & \text{O} \end{array} \right]^{8-}$ tetradecaaxo-2,5,7-trioxa-1,3,4,6,8,9-hexaphosphanonahetranate(8-)
11. $\left[\begin{array}{ccccccc} \text{O} & \text{O} & \text{O} & \text{O} & \text{O} & \text{O} & \text{O} \\ \text{OP}-\text{O}-\text{P}-\text{P}-\text{O}-\text{P}-\text{P}-\text{O}-\text{PO} \\ \text{O} & \text{O} & \text{O} & \text{O} & \text{O} & \text{O} & \text{O} \end{array} \right]^{8-}$ tetradecaaxo-2,5,8-trioxa-1,3,4,6,7,9-hexaphosphanonahetranate(8-)
or (4- μ)-oxo-bis(heptaoxo-2-oxa-1,3,4-triphosphatetrahtranate)(8-)
12. $\left[\begin{array}{ccccccc} \text{O} & \text{O} & \text{O} & \text{O} & \text{O} & \text{O} & \text{O} \\ \text{OP}-\text{P}-\text{O}-\text{P}-\text{O}-\text{P}-\text{O}-\text{P}-\text{PO} \\ \text{O} & \text{O} & \text{O} & \text{O} & \text{O} & \text{O} & \text{O} \end{array} \right]^{8-}$ tetradecaaxo-3,5,7-trioxa-1,2,4,6,8,9-hexaphosphanonahetranate(8-)
or (4- μ)-oxo-bis(heptaoxo-3-oxa-1,2,4-triphosphatetrahtranate)(8-)
13. $[\text{O}_3\text{S}-\text{O}-\text{Se}-\text{O}-\text{SO}_3]^{2-}$ 1,1,1,5,5,5-hexaoxo-2,4-dioxa-1,5-dithia-3-selenapentahetranate(2-)
14. $[\text{O}_3\text{S}-\text{S}-\text{S}-\text{S}-\text{SO}_3]^{2-}$ 1,1,1,5,5,5-hexaoxopentasulfanate(2-) (= pentathionate)
15. $[\text{O}_3\text{Se}-\text{O}-\text{CrO}_2-\text{O}-\text{SO}_3]^{4-}$ octaoxo-2,4-dioxa-1-thia-3-chroma-5-selenapentahetranate(4-)
16. $\left[\begin{array}{c} \text{O}_2 \\ \text{O}_2\text{P} \quad \text{P} \quad \text{PO}_2 \\ | \quad \quad | \\ \text{O}_2\text{P} \quad \text{P} \quad \text{PO}_2 \\ | \quad \quad | \\ \text{O}_2 \end{array} \right]^{6-}$ dodecaoxocyclohexaphosphanate
17. $\left[\begin{array}{c} \text{O}_2 \\ \text{O} \quad \text{P} \quad \text{O} \\ | \quad \quad | \\ \text{O}_2\text{P} \quad \text{PO}_2 \\ | \quad \quad | \\ \text{O} \end{array} \right]^{3-}$ hexaoxocyclotriphosphoxanate(3-)
(= *cyclo*-triphosphate)
18. $\left[\begin{array}{c} \text{O}_2\text{P} \quad \text{S} \quad \text{PO}_2 \\ | \quad \quad | \\ \text{HN} \quad \text{P} \quad \text{NH} \\ | \quad \quad | \\ \text{O}_2 \end{array} \right]^{3-}$ 2,2,4,4,6-hexaoxo-1-thia-3,5-diaza-2,4,6-triphosphacyclohexahetranate(3-)



octaoxo-1,4-dioxa-2,3-diphospha-5,6-diarsacyclohexahetranate(4-)

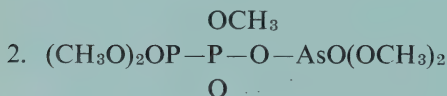
5.32 Names of the free acids and esters may be formed either a) as if they were salts by prefixing the word hydrogen or the name of the organic radical (with the necessary numerical prefixes) to the name of the anion, or b) as hydroxy or alkoxy derivatives of hydrides.

Examples



a) tetrahydrogen 1,1,1,2,3,3,3-hepta-oxo-2-hydridotriphosphanate

b) 1,1,3,3-tetrahydroxy-1,2,3-trioxotri-P(V)-phosphane



a) pentamethyl octaoxo-1-arsa-2-oxa-3,4-diphosphatetrahetrinate

b) 1,1,3,4,4-pentamethoxy-1,3,4-trioxo-2-oxa-(3,4)P(V)-diphospha-1As(V)-arsatetrahetrane

TENTATIVE

ADDENDUM TO: RULES ON COORDINATION COMPOUNDS^o

7.35

 π -Complexes

Compounds in which a bond from the centre of coordination is directed toward an existing bond in the ligand rather than toward a specific atom are often called π -complexes because the electrons constituting a π -bond in the ligand are also involved in the coordination bond.

7.351 A group bound by π -electrons as noted above is indicated by adding the Greek letter π immediately before its name. Where more than one double bond is present, π without modification implies the involvement of all double bonds in coordination.

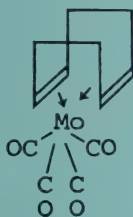
Examples

amminedichloro- π -ethyleneplatinum
amminedichloro- π -ethyleneplatinum(II)



potassium trichloro- π -ethyleneplatinate(I-)
potassium trichloro- π -ethyleneplatinate(II)

3.



tetracarbonyl- π -1,5-cyclooctadiene-
molybdenum
tetracarbonyl- π -1,5-cyclooctadiene-
molybdenum(0)

4.

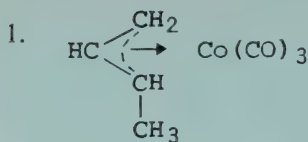


tricarbonyl- π -bicyclo[2.2.1]heptadieneiron
tricarbonyl- π -bicyclo[2.2.1]heptadieneiron(0)

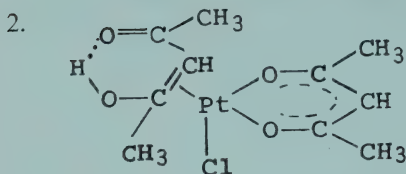
7.352 The π -electrons involved in binding the group to a centre of coordination may encompass more than two atoms. In such a case, the atoms involved are indicated by number locants.

^o Comments should be sent to the chairman of the Commission, Prof. K. A. JENSEN, Chemical Laboratory II of the University of Copenhagen, The H. C. Ørsted Institute, Universitetsparken 5, 2100 Copenhagen Ø.

Examples



tricarbonyl- $\pi(1-3)$ -butenylcobalt
tricarbonyl- $\pi(1-3)$ -butenylcobalt(I)



chloro- $\pi(2-3)$ -(2-hydroxy-2-pentene-4-one)-
2,4-pentandionatoplatinum
chloro- $\pi(2-3)$ -(2-hydroxy-2-pentene-4-one)-
2,4-pentandionatoplatinum(II)

7.353 When the π -electrons involved in binding a group to a center of coordination extend around a complete ring or through a conjugated double bond, locants are unnecessary.

Examples

- | | |
|--|---|
| 1. $[\text{Cr}(\text{C}_6\text{H}_6)_2]$ | di- π -benzenechromium
di- π -benzenechromium(0) |
| 2. $[\text{Ni}(\text{C}_5\text{H}_5)_2]$ | di- π -cyclopentadienylnickel
di- π -cyclopentadienylnickel(II) |
| 3. $[\text{ReH}(\text{C}_5\text{H}_5)_2]$ | di- π -cyclopentadienylhydridorhenium
di- π -cyclopentadienylhydridorhenium(I) |
| 4. $[\text{Cr}(\text{CO})_3(\text{C}_6\text{H}_6)]$ | π -benzenetricarbonylchromium
π -benzenetricarbonylchromium(0) |
| 5. $[\text{Co}(\text{C}_5\text{H}_5)(\text{C}_5\text{H}_6)]$ | π -cyclopentadiene- π -cyclopentadienylcobalt
π -cyclopentadiene- π -cyclopentadienylcobalt(I) |
| 6. $[\text{Ni}(\text{C}_5\text{H}_5)(\text{NO})]$ | π -cyclopentadienylnitrosylnickel |

7.354 The general term for π -cyclopentadienyl complexes and their derivatives is *metallocenes*. The trivial name for di- π -cyclopentadienyliron, $\text{Fe}(\text{C}_5\text{H}_5)_2$, is ferrocene.

Note

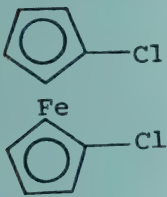
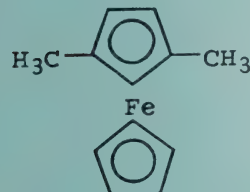
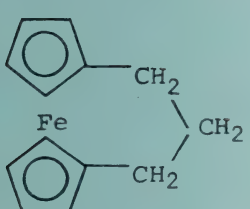
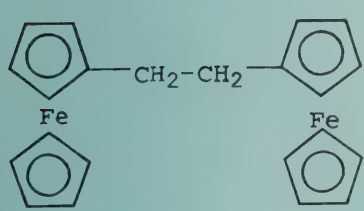
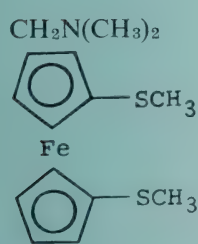
The term “sandwich compounds” is too general to be used to designate the metallocenes specifically. “Ocene” names (nickelocene, cobaltocene, osmocene, etc.) should not be employed for individual compounds (at least, as long as their organic chemistry is not as well developed as that of ferrocene). The introduction of other trivial names, such as cymantrene and tizel similarly should be avoided.

Examples

- | | |
|---|--|
| 1. $\text{Fe}(\text{C}_5\text{H}_5)_2$ | di- π -cyclopentadienyliron
di- π -cyclopentadienyliron(II)
ferrocene |
| 2. $[\text{Fe}(\text{C}_5\text{H}_5)_2][\text{BF}_4]$ | di- π -cyclopentadienyliron(1+) tetrafluoroborate(1—)
di- π -cyclopentadienyliron(III) tetrafluoroborate
ferrocene(1+) tetrafluoroborate(1—) |

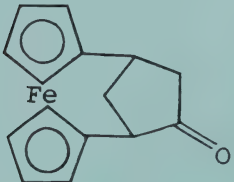
7.355 Derivatives of ferrocene are named by the use of the prefixes and suffixes for organic substituents. However, any substituent may be indicated by a prefix (see 7.356). Since all of the positions on the cyclopentadiene rings may be considered equivalent, substituents are given low numbering without regard to attachment of the iron. The second cyclopentadiene ring is numbered with primed numbers: 1', 2', etc. If the compound contains two ferrocene groups, doubly and triply primed numbers (1'', 1''', etc.) are used for the third and fourth cyclopentadienyl group.

Examples

1.  1, 1'-dichloroferrocene
2.  1, 3-dimethylferrocene
3.  1, 1'-trimethyleneferrocene
4.  1, 1''-ethylenediferrocene
5. $\text{CH}_2\text{N}(\text{CH}_3)_2$
 3-[(dimethylamino)methyl]-1, 1'-bis(methylthio)-ferrocene
or
N,N-dimethyl-1', 3-bis(methylthio)-1-ferrocene-methylamine (see 7.356)
6. $[\text{Fe}(\text{C}_2\text{H}_5\text{C}_5\text{H}_4)(\text{C}_5\text{H}_5)]\text{Cl}$ ethylferrocene(1 +) chloride

7.356 (in part alternate to 7.355). Ferrocene derivatives containing a principal group which can be designated by a suffix may alternatively be named as an organic parent compound with a ferrocene radical as substituent. When necessary, radical names such as ferrocenyl, ferrocenediyl, and ferrocenetriyl are used.

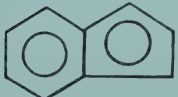
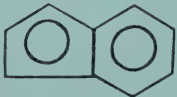
Examples

- | | |
|---|---|
| 1. $(C_{10}H_9Fe)-COCH_3$ | ferrocenylmethylketone
or
acetylferrocene |
| 2. $(C_{10}H_9Fe)-CHO$ | ferrocenecarbaldehyde
or
formylferrocene |
| 3. $(C_{10}H_9Fe)-CH_2OH$ | ferrocenylmethanol
or
hydroxymethylferrocene |
| 4. $(C_{10}H_9Fe)-COOH$ | ferrocenecarboxylic acid
or
carboxyferrocene |
| 5. $(C_{10}H_9Fe)-CH_2CHNH_2COOH$ | α -aminoferrocenepropionic acid
or
β -ferrocenylalanine |
| 6. $(C_{10}H_9Fe)-As(C_6H_5)_2$ | ferrocenyldiphenylarsine
or
(diphenylarsino)ferrocene |
| 7. $(C_{10}H_9Fe)_2NC_2H_5$ | <i>N</i> -ethyl-1,1''-diferrocenylamine
or
1,1'-(ethylimino)diferrocene |
| 8. $(C_{10}H_9Fe)-\overset{+}{N}(CH_3)_3$ | ferrocenyltrimethylammonium
or
(trimethylammonio)ferrocene |
| 9. | |
|  | 2,4-(ferrocene-1,1'-diyl)-cyclopentanone |

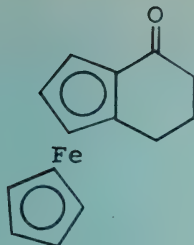
Note

The above treatment is not extended to ferrocene derivatives of more complex ring structures than cyclopentadiene.

Examples

- | | | | |
|-----|--|---|---|
| 10. |  |  | di- π -1-indenyliron (not benzoferrocene or dibenzoferrocene) |
|-----|--|---|---|

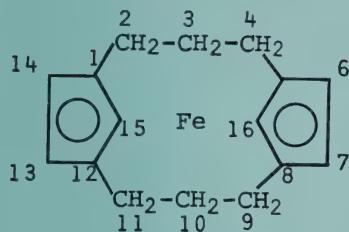
11.



π -cyclopentadienyl- π -(4,5,6,7-tetrahydro-4-oxoindenyl)iron

π -cyclopentadienyl- π -(4,5,6,7-tetrahydro-4-oxoindenyl)iron(II)

12.

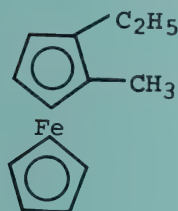


tricyclo[10.2.1.1^{5,8}]hexadecatetraenyliron

7.357. The absolute configuration of enantiomers is specified by the sequence-rule method (*cf.* R. S. CAHN / Sir CHRISTOPHER INGOLD / V. PRELOG: *Angew. Chem. Internat. Ed.* 5 (1966), p. 394: Convention for π -complexes).

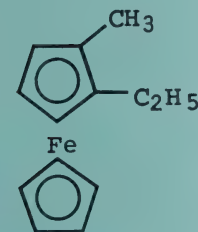
Examples:

1.



(1S)-ethyl-(2R)-methylferrocene

2.



(1R)-ethyl-(2S)-methylferrocene

IUPAC TENTATIVE RULES FOR THE NOMENCLATURE OF ORGANIC CHEMISTRY

Section E: Fundamental Stereochemistry[♦]

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Introduction

This Section of the IUPAC Rules for Nomenclature of Organic Chemistry differs from previous Sections in that it is here necessary to legislate for words that describe concepts as well as for names of compounds.

At the present time, concepts in stereochemistry (that is, chemistry in three-dimensional space) are in the process of rapid expansion, not merely in organic chemistry, but also in biochemistry, inorganic chemistry, and macromolecular chemistry. The aspects of interest for one area of chemistry often differ from those for another, even in respect of the same phenomenon. This rapid evolution and the variety of interests have led to development of specialized vocabularies and definitions that sometimes differ from one group of specialists to another, sometimes even within one area of chemistry.

The Commission on the Nomenclature of Organic Chemistry does not, however, consider it practical to cover all aspects of stereochemistry in this Section E. Instead, it has two objects in view: to prescribe, for basic concepts, terms that may provide a common language in all areas of stereochemistry; and to define the ways in which these terms may, so far as necessary, be incorporated into the names of individual compounds. The Commission recognizes that specialized nomenclatures are required for local fields; in some cases, such as carbohydrates, amino acids, peptides and pro-

[♦] These Rules may be called the IUPAC 1968 Tentative Rules, Section E, Fundamental Stereochemistry. They are issued by the Commission^{♦♦} on the Nomenclature of Organic Chemistry of the International Union of Pure and Applied Chemistry. Section A: Hydrocarbons, and Section B: Fundamental Heterocyclic Systems, were published in 1957 (2nd edition, 1966); Section C: Characteristic Groups Containing Carbon, Hydrogen, Oxygen, Nitrogen, Halogen, Sulfur, Selenium, and/or Tellurium, was published in 1965. Section D, which is in preparation and is expected to be published soon, will deal with organometallic compounds in general, chains and rings containing heterogeneous atoms, and organic derivatives of phosphorus, arsenic, antimony, bismuth, silicon, and boron. Comments on Section E should be addressed to the Secretary of the Commission named in the following footnote.

^{♦♦} Titular members: P.E. VERKADE (Chairman), S.P. KLESNEY (Secretary, 3609 Boston, Midland, Michigan 48640, USA), L.C. CROSS, G.M. DYSON, K.L. LOENING, N. LOZACH, H.S. NUTTING, J. RIGAUDY, S. VEIBEL. Associate members: R.S. CAHN, H. GRÜNEWALD. Observers: K.A. JENSEN, W. KLYNE.

teins, and steroids, international rules already exist; for other fields, study is in progress by specialists in Commissions or Sub-Committees; and further problems doubtless await identification. The Commission believes that consultations will be needed in many cases between different groups within IUPAC and IUB if the needs of the specialists are to be met without confusion and contradiction between the various groups.

The Rules in this Section deal only with Fundamental Stereochemistry, that is, the main principles. Many of these Rules do little more than codify existing practice, often of long standing; however, others extend old principles to wider fields, and yet others deal with nomenclature that is still subject to controversy.

RULES

Rule E-0

The stereochemistry of a compound is denoted by an affix or affixes to the name that does not prescribe the stereochemistry; such affixes, being additional, do not change the name or the numbering of the compound. Thus, enantiomers, diastereoisomers, and *cis-trans*-isomers receive names that are distinguished only by means of different stereochemical affixes. The only exceptions are those trivial names that have stereochemical implications (for example, fumaric acid, cholesterol).

Note: In some cases (see Rules E-2.23 and E-3.1) stereochemical relations may be used to decide between alternative numberings that are otherwise permissible.

E-1 Types of Isomerism

E-1.1 The following non-stereochemical terms are relevant to the stereochemical nomenclature given in the Rules that follow:

(a) The term structure may be used in connexion with any aspect of the organization of matter.

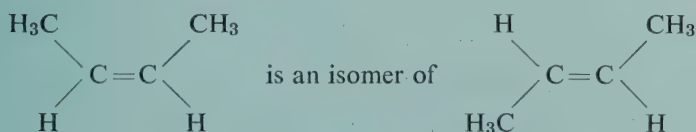
Hence: structural (adjectival)

(b) Compounds that have identical molecular formulae but differ in the nature or sequence of bonding of their atoms or in arrangement of their atoms in space are termed isomers.

Hence: isomeric (adjectival)
isomerism (phenomenological)

Examples:

$\text{H}_3\text{C}-\text{O}-\text{CH}_3$ is an isomer of $\text{H}_3\text{C}-\text{CH}_2-\text{OH}$



(In this and other Rules a broken line denotes a bond projecting behind the plane of the paper, and a thickened line denotes a bond projecting in front of the plane of the paper. In such cases a line of normal thickness denotes a bond lying in the plane of the paper.)

(c) The constitution of a compound of given molecular formula defines the nature and sequence of bonding of the atoms. Isomers differing in constitution are termed constitutional isomers.

Hence: constitutionally isomeric (adjectival)
constitutional isomerism (phenomenological)

Example:

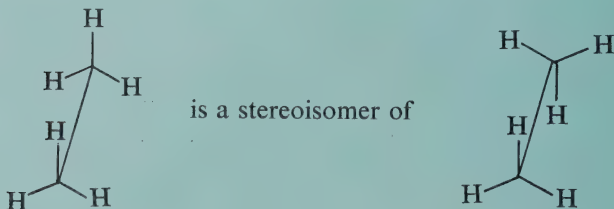
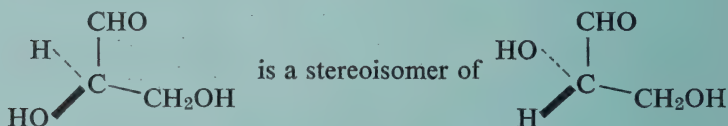
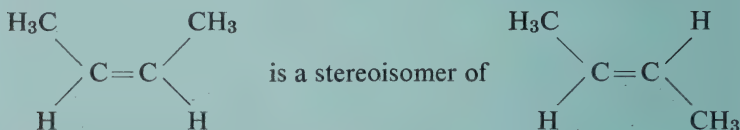
$\text{H}_3\text{C}-\text{O}-\text{CH}_3$ is a constitutional isomer of $\text{H}_3\text{C}-\text{CH}_2-\text{OH}$

Note: Use of the term “structural” with the above connotation is abandoned as insufficiently specific.

E-1.2 Isomers are termed stereoisomers when they differ only in the arrangement of their atoms in space.

Hence: stereoisomeric (adjectival)
stereoisomerism (phenomenological)

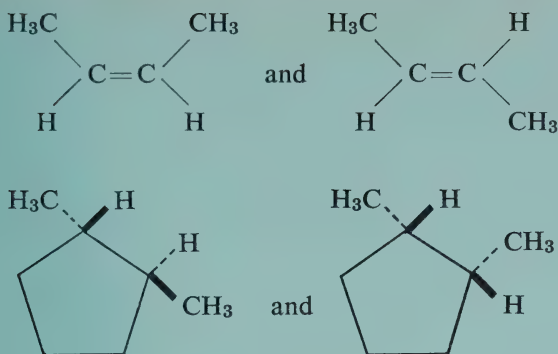
Examples:



E-1.3 Stereoisomers are termed *cis-trans*-isomers when they differ only in the positions of atoms relative to a specified plane in cases where these atoms are, or are considered as if they were, parts of a rigid structure.

Hence: *cis-trans*-isomeric (adjectival)
cis-trans-isomerism (phenomenological)

Examples:



E-1.4 Various views are current regarding the precise definition of the term “configuration”. (a) Classical interpretation: The configuration of a molecule of defined constitution is the arrangement of its atoms in space without regard to arrangements that differ only as after rotation about one or more single bonds. (b) This definition is now usually limited so that no regard is paid also to rotation about π -bonds or bonds of partial order between one and two. (c) A third view limits the definition further so that no regard is paid to rotation about bonds of any order, including double bonds.

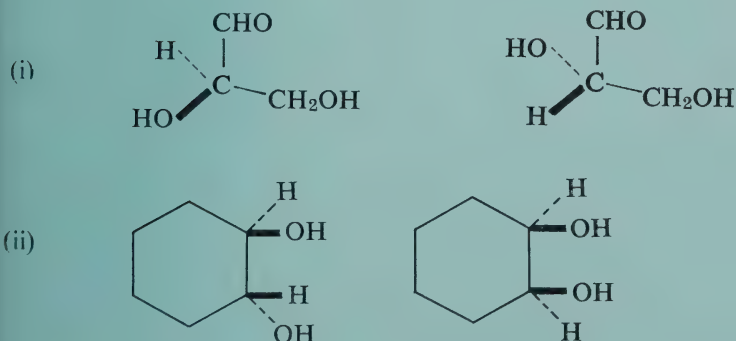
Molecules differing in configuration are termed configurational isomers.

Hence: configurational isomerism

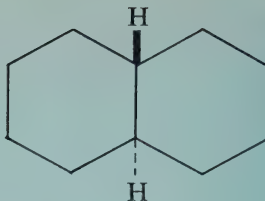
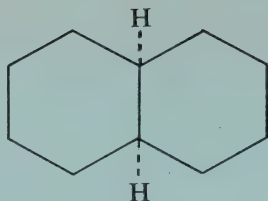
- Notes: (1) Contrast Conformation (Rule E-1.5).
 (2) The phrase “differ only as after rotation” is intended to make the definition independent of any difficulty of rotation, in particular independent of steric hindrance to rotation.
 (3) For a brief discussion of views (a)–(c) see Appendix 1. It is hoped that a definite consensus of opinion will be established before these Rules are made “Definitive”.

Examples:

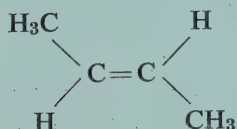
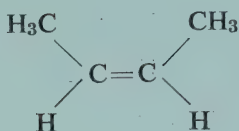
The following pairs of compounds differ in configuration:



(iii)



(iv)



These isomers (iv) are configurational in view (a) or (b) but are conformational (see Rule E-1.5) in view (c)

E-1.5

Various views are current regarding the precise definition of the term "conformation". (a) Classical interpretation: The conformations of a molecule of defined configuration are the various arrangements of its atoms in space that differ only as after rotation about single bonds. (b) This is usually now extended to include rotation about π -bonds or bonds of partial order between one and two. (c) A third view extends the definition further to include also rotation about bonds of any order, including double bonds.

Molecules differing in conformation are termed conformational isomers.

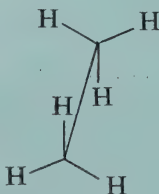
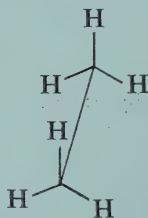
Hence: conformational isomerism

Notes: All the Notes to Rule E-1.4 apply also to E-1.5.

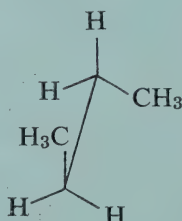
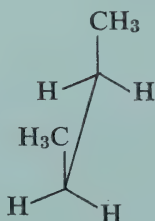
Examples:

Each of the following pairs of formulae represents a compound in the same configuration but in different conformations.

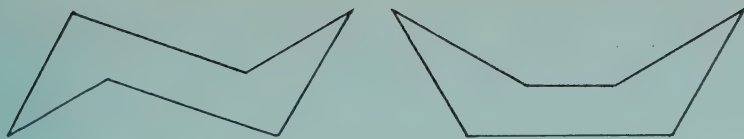
(a, b, c)



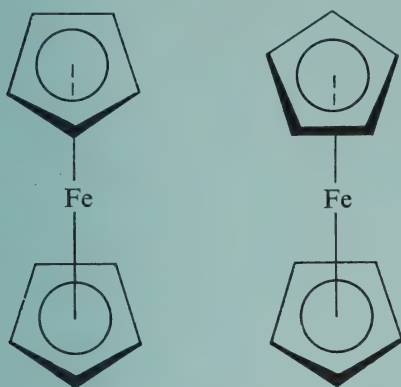
(a, b, c)



(a, b, c)



(b, c)



(c) See Example (iv) to Rule E-1.4.

E-1.6 The terms relative stereochemistry and relative configuration are used with reference to the positions of various atoms in a compound relative to one another, especially, but not only, when the actual positions in space (absolute configuration) are unknown.

E-1.7 The terms absolute stereochemistry and absolute configuration are used with reference to the known actual positions of the atoms of a molecule in space.

E-2 *cis-trans-Isomerism*⁴⁰

Preamble:

The prefixes *cis* and *trans* have long been used for describing the relative positions of atoms or groups attached to non-terminal doubly bonded atoms of a chain or attached to a ring that is considered as planar. This practice has been codified for hydrocarbons by IUPAC (see footnote ⁴⁰below). There has, however, not been agreement on how to assign *cis* or *trans* at terminal double bonds of chains or at double bonds joining a chain to a ring. An obvious solution was to use *cis* and *trans* where doubly bonded atoms formed the backbone and were non-terminal and to enlist the sequence-rule preferences to decide other cases; however, since the two methods, when generally applied, do not always produce analogous results, it would then be necessary to use different symbols for the two procedures. A study of this combination showed that both types of symbol would often be required in one name and, moreover, it seemed wrong in principle to use two symbolisms for essentially

⁴⁰ Determination of absolute configuration became possible through work by J.M.BIJVOET, A.F.PEERDEMAN, and A.J. VAN BOMMEL: *Nature* 168, 271 (1951); cf. J.M.BIJVOET: *Proc.Kon. Ned. Akad. Wet. Amsterdam* 52, 313 (1949).

⁴¹ These Rules supersede the Tentative Rules for olefinic hydrocarbons published in the Comptes rendus of the 16th IUPAC Conference, New York, 1951, pages 102-103.

the same phenomenon. Thus it seemed to the Commission wise to use only the sequence-rule system, since this alone was applicable to all cases. The same decision was taken independently by *Chemical Abstracts Service*⁸ who introduced *Z* and *E* to correspond more conveniently to *seqcis* and *seqtrans* of the sequence rule.

It is recommended in the Rules below that these designations *Z* and *E* based on the sequence rule shall be used in names of compounds; but *Z* and *E* do not always correspond to the classical *cis* and *trans* which show the steric relations of like or similar groups that are often the main point of interest. So the use of *Z* and *E* in names is not intended to hamper the use of *cis* and *trans* in discussions of steric relations of a generic type or of groups of particular interest in a specified case (see Rule E-2.1 and its Examples and Notes, also Rule E-5.11).

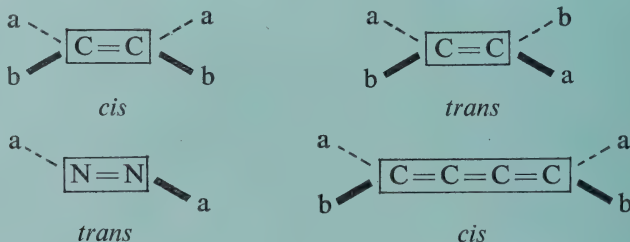
It is also not necessary to replace *cis* and *trans* for describing the stereochemistry of substituted monocycles (see Subsection E-3). For cyclic compounds the main problems are usually different from those around double bonds; for instance, steric relations of substituents on rings can often be described either in terms of chirality (see Subsection E-5) or in terms of *cis-trans*-relationships, and, further, there is usually no single relevant plane of reference in a hydrogenated polycycle. These matters are discussed in the Preambles to Subsections E-3 and E-4.

E-2 Definition of *cis-trans*

E-2.1 Atoms or groups are termed *cis* or *trans* to one another when they lie respectively on the same or on opposite sides of a reference plane identifiable as common among stereoisomers. The compounds in which such relations occur are termed *cis-trans*-isomers. For compounds containing only doubly bonded atoms the reference plane contains the doubly bonded atoms and is perpendicular to the plane containing these atoms and those directly attached to them. For cyclic compounds the reference plane is that in which the ring skeleton lies or to which it approximates. When qualifying another word or a locant, *cis* or *trans* is followed by a hyphen. When added to a structural formula, *cis* may be abbreviated to *c*, and *trans* to *t* (see also Rule E-3.3).

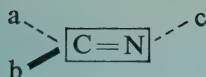
Examples:

[Rectangles here denote the reference planes and are considered to lie in the plane of the paper.]

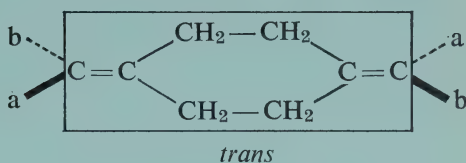
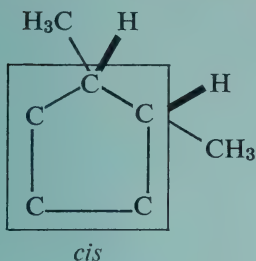


The groups or atoms *a, a* are the pair selected for designation but are not necessarily identical; *b, b* are also not necessarily identical but must be different from *a, a*.

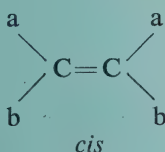
♦ J.E.BLACKWOOD, C.L.GLADYS, K.L.LOENING, A.E.PETRARCA, and J.E.RUSH: *J. Amer. Chem. Soc.* 90, 509 (1968); J.E.BLACKWOOD, C.L.GLADYS, A.E.PETRARCA, W.H.POWELL, and J.E.RUSH: *J. Chem. Document.* 8, 30 (1968).



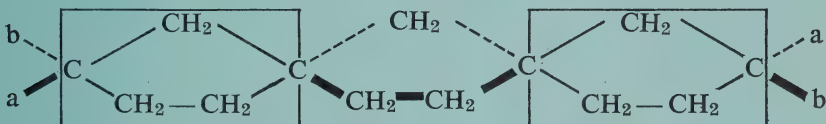
cis or *trans* according as a or b is taken as basis of comparison



Notes: The formulae above are drawn with the reference plane in the plane of the paper, but for doubly bonded compounds it is customary to draw the formulae so that this plane is perpendicular to that of the paper; atoms attached directly to the doubly bonded atoms then lie in the plane of the paper and the formulae appear as, for instance:

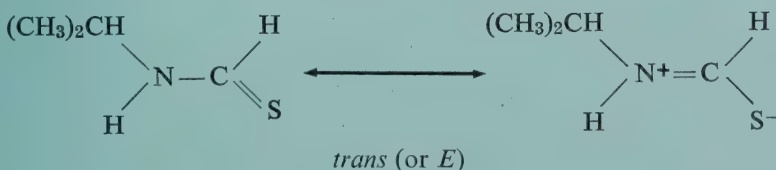


Cyclic structures, however, are customarily drawn with the ring atoms in the plane of the paper, as above. However, care is needed for complex cases, such as:



The central five-membered ring lies (approximately) in a plane perpendicular to the plane of the paper. The two *a* groups are *trans* to one another; so are the *b* groups; the outer cyclopentane rings as *cis* to one another with respect to the plane of the central ring.

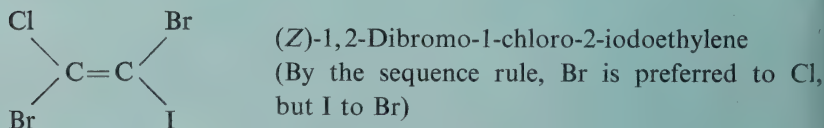
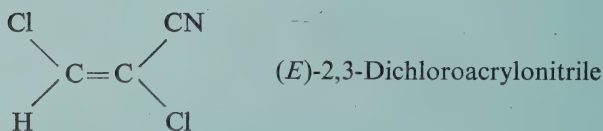
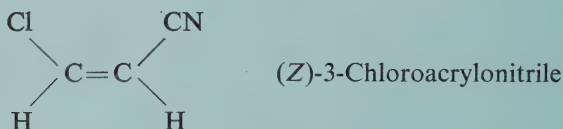
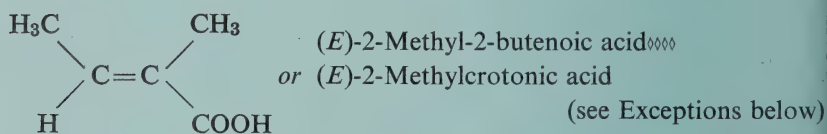
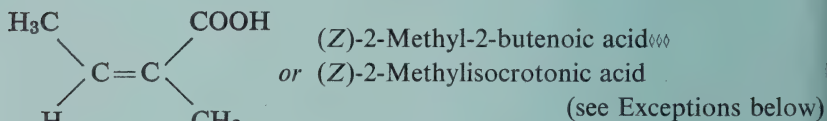
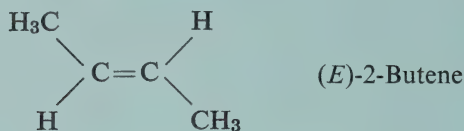
cis or *trans* (or *Z* or *E*; see Rule E-2.21) may also be used in cases involving a partial bond order when a limiting structure is of sufficient importance to impose rigidity around the bond of partial order. An example is:



E-2.2 *cis-trans*-Isomerism around double bonds

E-2.21 In names of compounds steric relations around one or more double bonds are designated by affixes *Z* and/or *E*, assigned as follows. The sequence-rule-preferred[◇] atom or group attached to one of a doubly bonded pair of atoms is compared with the sequence-rule-preferred atom or group attached to the other of that doubly bonded pair of atoms; if the selected pair are on the same side of the reference plane (see Rule 2.1) an italic capital letter *Z* prefix is used; if the selected pair are on opposite sides an italic capital letter *E* prefix is used^{◇◇}. These prefixes, placed in parentheses and followed by a hyphen, normally precede the whole name; if the molecule contains several double bonds, then each prefix is immediately preceded by the lower or less primed locant of the relevant double bond.

Examples:

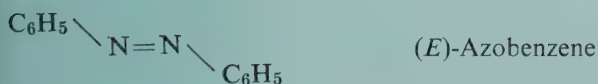
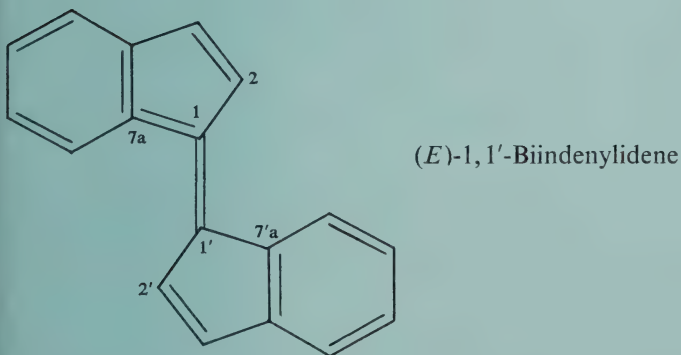
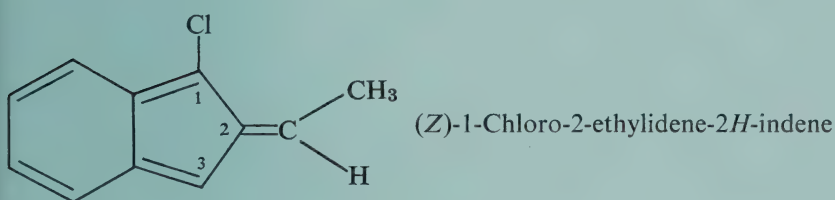
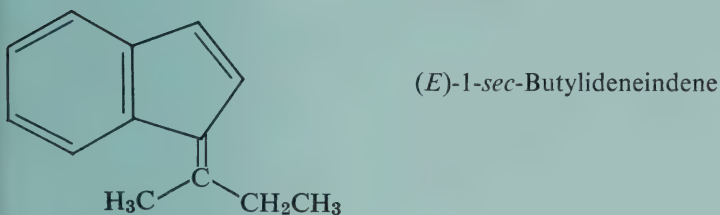
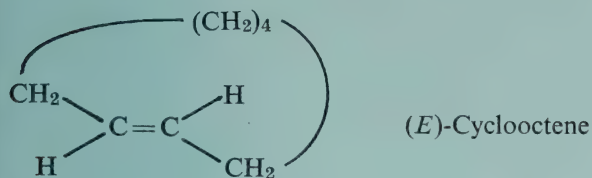
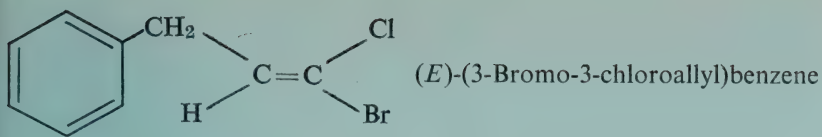


[◇] For sequence-rule preferences see Appendix 2.

^{◇◇} These prefixes may be rationalized as from the German *zusammen* (together) and *entgegen* (opposite).

^{◇◇◇} The name angelic acid is abandoned because it has been associated with the designation *trans* with reference to the methyl groups.

^{◇◇◇◇} The name tiglic acid is abandoned because it has been associated with the designation *cis* with reference to the methyl groups.



Exceptions to Rule E-2.21:

The following are examples of accepted trivial names in which the stereochemistry is prescribed by the name and is not cited by a prefix:

$\begin{array}{c} \text{HOOCCH} \\ \\ \text{HCCOOH} \end{array}$	Fumaric acid
$\begin{array}{c} \text{HCCOOH} \\ \\ \text{HCCOOH} \end{array}$	Maleic acid
$\begin{array}{c} \text{CH}_3\text{CCOOH} \\ \\ \text{HCCOOH} \end{array}$	Citraconic acid \diamond
$\begin{array}{c} \text{HOOCCCH}_3 \\ \\ \text{HCCOOH} \end{array}$	Mesaconic acid \diamond
$\begin{array}{c} \text{CH}_3\text{CH} \\ \\ \text{HCCOOH} \end{array}$	Crotonic acid
$\begin{array}{c} \text{HCCH}_3 \\ \\ \text{HCCOOH} \end{array}$	Isocrotonic acid
$\begin{array}{c} \text{HC}-(\text{CH}_2)_7-\text{CH}_3 \\ \\ \text{HC}-(\text{CH}_2)_7-\text{COOH} \end{array}$	Oleic acid
$\begin{array}{c} \text{CH}_3-(\text{CH}_2)_7-\text{CH} \\ \\ \text{HC}-(\text{CH}_2)_7-\text{COOH} \end{array}$	Elaidic acid

E-2.22 (Alternative to part of E-2.21)

(a) When more than one series of locants starting from unity is required to designate the double bonds in a molecule, or when the name consists of two words, the *Z* and *E* prefixes together with their appropriate locants may be placed before that part of the name where ambiguity is most effectively removed.

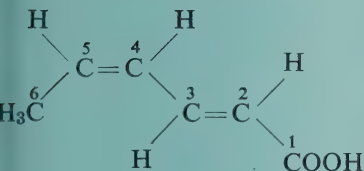
(b) [Alternative to (a)] When several *Z* or *E* prefixes are required they are arranged in order as follows: of the four atoms or groups attached to each doubly bonded pair of atoms, that one preferred by the sequence rule is selected; the single atoms or groups thus selected are then arranged in their sequence rule order (determined in respect of their position in the whole molecule), and the prefixes *Z* and/or *E* for the respective double bonds are placed in that order, but *without* their locants.

Note: In method (a) the final choice is left to an author or editor because of the variety of cases met and because the problems are not always the

\diamond Systematic names are recommended for derivatives of these compounds formed by substitution on carbon.

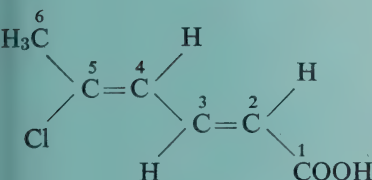
same in different languages. Presence of the locants usually eases translation from the name to a formula, but this method (a) may involve the logical difficulty explained for the third example below. Method (b) always gives a single unambiguous order and is not subject to the logical difficulty just mentioned, but translation from the name to the formula is harder than for method (a). Method (a) may be more suitable for cursive text, and method (b) for compendia. If method (b) is used it should be used whenever more than one double bond is involved; but method (a) is to be used only under the special conditions detailed in the rule.

Examples:



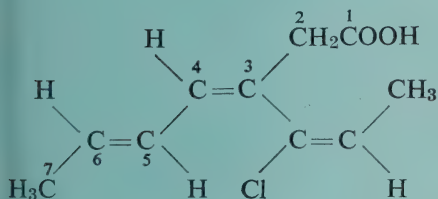
(a) (2*E*,4*Z*)-2,4-Hexadienoic acid

(b) (*E*,*Z*)-2,4-Hexadienoic acid



(a) (2*E*,4*Z*)-5-Chloro-2,4-hexadienoic acid

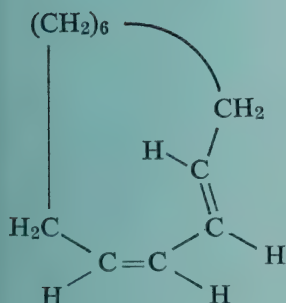
(b) (*Z*,*E*)-5-Chloro-2,4-hexadienoic acid



(a) 3-[(*E*)-1-Chloropropenyl]-(3*Z*,5*E*)-3,5-heptadienoic acid

(b) (*E*,*Z*,*E*)-3-(1-Chloropropenyl)-3,5-heptadienoic acid

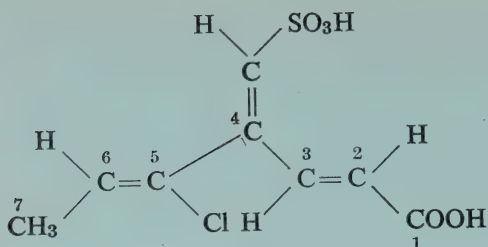
[The last example shows the disadvantages of both methods. In method (a) there is a fault of logic, namely, the 3*Z*,5*E* are not the property of the unsubstituted heptadienoic acid chain, but the 3*Z* arises only because of the side chain that is cited before the 3*Z*,5*E*. In method (b) it is some trouble to assign the *E*, *Z*, *E* to the correct double bonds.]



(a) (1*Z*,3*E*)-1,3-Cyclododecadiene

(b) (*Z*,*E*)-1,3-Cyclododecadiene

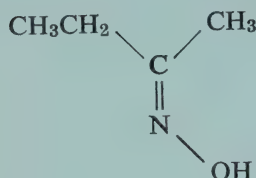
[The lower locant is assigned to the *Z* double bond.]



(a) 5-Chloro-4-(*E*-sulfomethylene)-
(2*E*,5*Z*)-2,5-heptadienoic acid

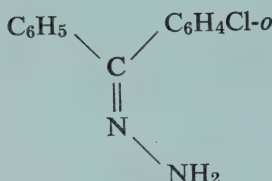
(b) (*Z*,*E*,*E*)-5-Chloro-4-(sulfo-
methylene)-2,5-heptadienoic acid

[In application of the sequence rule, the relation of the SO₃H to CCl (rather than to C-3), and of the CH₃ to Cl, are decisive.]



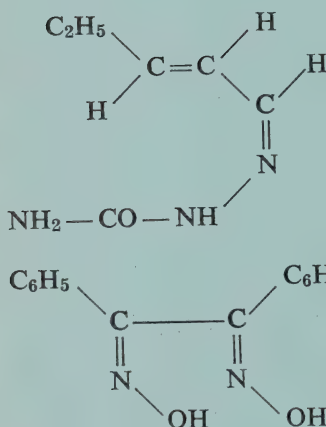
(a) Butanone (*E*)-oxime

(b) (*E*)-Butanone oxime



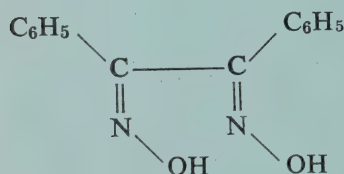
(a) 2-Chlorobenzophenone (*Z*)-hydrazone

(b) (*Z*)-2-Chlorobenzophenone hydrazone



(a) (*E*)-2-Pentenal (*Z*)-semicarbazone

(b) (*Z*,*E*)-2-Pentenal semicarbazone

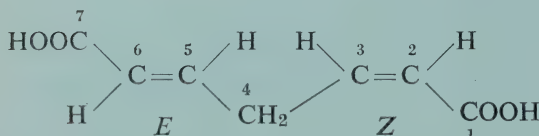


(a) Benzil (*Z*,*E*)-dioxime

(b) (*Z*,*E*)-Benzil dioxime

E-2.23 When Rule C-13.1 or E-2.22(b) permits alternatives, preference for lower locants and for inclusion in the principal chain is allotted as follows, in the order stated, so far as necessary: *Z* over *E* groups; *cis* over *trans* cyclic groups; *R* over *S* groups (also *r* over *s*, etc., as in the sequence rule); if the nature of these groups is not decisive, then the lower locant for such a preferred group at the first point of difference.

Examples:

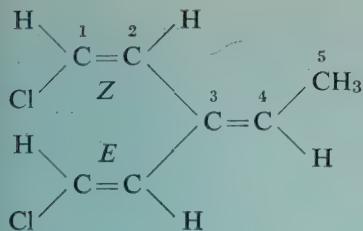


(a) (2*Z*,5*E*)-2,5-Heptadienedioic acid

(b) (*Z*,*E*)-2,5-Heptadienedioic acid

[The lower numbers are assigned to the *Z* double bond.]

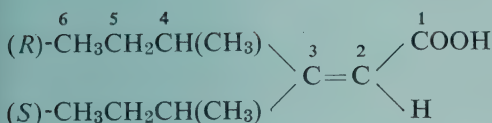
† The terms *syn*, *anti*, and *amphi* are abandoned for such compounds.



(a) 1-Chloro-3-[2-chloro-(*E*)-vinyl]-(1*Z*,3*Z*)-1,3-pentadiene

(b) (*Z,E,Z*)-1-Chloro-3-(2-chlorovinyl)-1,3-pentadiene

[According to Rule C-13.1 the principal chain must include the C=C—CH₃ group because this gives lower numbers to the double bonds (1,3 rather than 1,4); then the Cl-containing *Z* group is chosen for the remainder of the principal chain in accord with Rule E-2.23.]



(a, b) (*Z*)-(4*R*)-[3(*S*)-*sec*-Butyl]-4-methyl-2-hexenoic acid

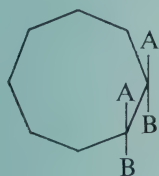
[The principal chain is chosen to include the (*R*)-group, and the prefix *Z* refers to the (*R*)-group.]

E-3 Relative Stereochemistry of Substituents in Monocyclic Compounds[♦]

Preamble:

cis- and *trans*-Prefixes are commonly used to designate the positions of substituents on rings relative to one another; when the ring is, or is considered to be, rigidly planar or approximately so and is placed horizontally, these prefixes define which groups are above and which below the (approximate) plane of the ring. This differentiation is often important, so this classical terminology is retained in Subsection E-3; since the difficulties inherent in end-groups do not arise for cyclic compounds it is unnecessary to resort to the less immediately informative *E/Z* symbolism.

When the *cis-trans*-designation of substituents is applied, rings are considered in their most extended form; reentrant angles are not permitted; for example:



cis

and not



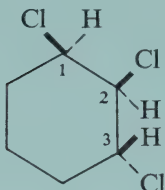
apparently *trans*

The absolute stereochemistry of optically active or racemic derivatives of monocyclic compounds is described by the sequence-rule procedure (see Rule E-5.9 and Appendix 2). The relative stereochemistry may be described by a modification of sequence-rule symbolism as set out in Rule E-5.10. If either of these procedures is adopted, it is then superfluous to use also *cis* or *trans* in the names of individual compounds.

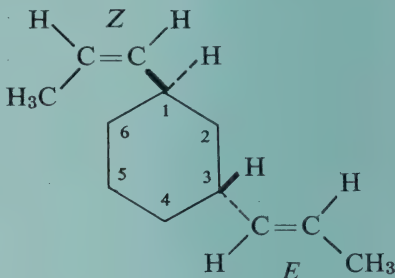
[♦] Formulae in Examples to this Rule denote relative (not absolute) configurations.

E-3.1 When alternative numberings of the ring are permissible according to the Rules of Section C, that numbering is chosen which gives a *cis* attachment at the first point of difference; if that is not decisive, the criteria of Rule E-2.23 are applied. *cis*- and *trans*- may be abbreviated to *c*- and *t*-, respectively, in names of compounds when more than one such designation is required.

Examples:



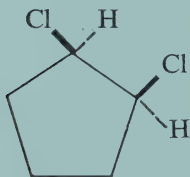
1, *c*-2, *t*-3-Trichlorocyclohexane



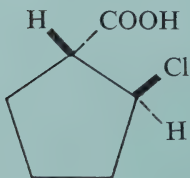
1-(*Z*)-Propenyl-*trans*-3-(*E*)-propenylcyclohexane

E-3.2 When one substituent and one hydrogen atom are attached at each of two positions of a monocycle, the steric relations of the two substituents are expressed as *cis* or *trans*, followed by a hyphen and placed before the name of the compound.

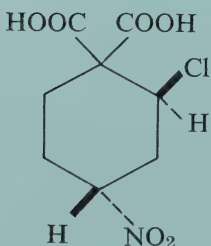
Examples:



cis-1,2-Dichlorocyclopentane



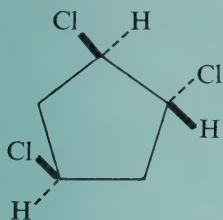
trans-2-Chloro-1-cyclopentanecarboxylic acid



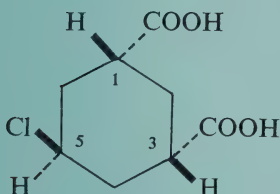
trans-2-Chloro-4-nitro-1,1-cyclohexanedicarboxylic acid

E-3.3 When one substituent and one hydrogen atom are attached at each of more than two positions of a monocycle, the steric relations of the substituents are expressed by adding *r* (for *reference* substituent), followed by a hyphen, before the locant of the lowest-numbered of these substituents and *c* or *t* (as appropriate), followed by a hyphen, before the locants of the other substituents to express their relation to the reference substituent.

Examples:



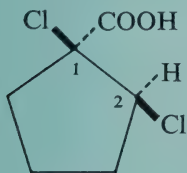
r-1, *t*-2, *c*-4-Trichlorocyclopentane
(not *r*-1, *t*-2, *t*-4 which would follow from the alternative direction of numbering; see Rule E-3.1)



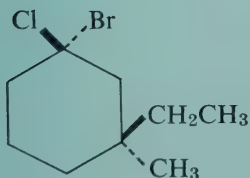
t-5-Chloro-*r*-1, *c*-3-cyclohexanedicarboxylic acid

E-3.4 When two different substituents are attached at the same position of a monocycle, then the lowest-numbered substituent named as suffix is selected for designation as reference group in accordance with Rule E-3.2 or E-3.3; or, if none of the substituents is named as suffix, then of the lowest-numbered pair that one preferred by the sequence rule is selected as reference group; and the relation of the sequence-rule preferred group at each other position, relative to the reference group, is cited as *c* or *t* (as appropriate).

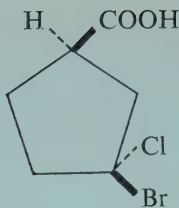
Examples:



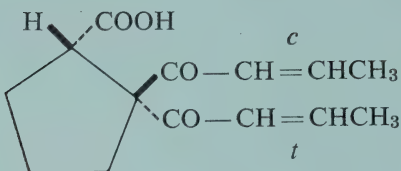
1, *t*-2-Dichloro-*r*-1-cyclopentanecarboxylic acid



r-1-Bromo-1-chloro-*t*-3-ethyl-3-methyl-cyclohexane (alphabetical order of prefixes)



c-3-Bromo-3-chloro-*r*-1-cyclopentanecarboxylic acid



2-Crotonoyl-*t*-2-isocrotonoyl-*r*-1-cyclopentanecarboxylic acid

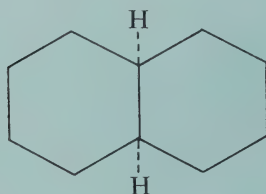
E-4 Fused Rings

Preamble:

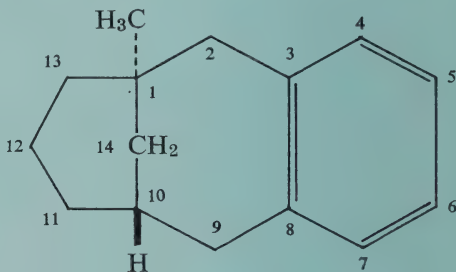
In simple cases the relative stereochemistry of substituted fused-ring systems can be designated by the methods used for monocycles. For the absolute stereochemistry of optically active and racemic compounds the sequence-rule procedure can be used in all cases (see Rule E-5.9 and Appendix 2); and for related relative stereochemistry the procedure of Rule E-5.10 can be applied. Sequence-rule methods are, however, not descriptive of geometrical shape for other than quite simple cases. There is as yet no generally acceptable system for designating in an immediately interpretable manner the stereochemistry of polycyclic bridged ring compounds (for instance, the *endo-exo* nomenclature, which should solve one set of problems, has been used in different ways). These and related problems (*e.g.*, cyclophanes, catenanes) will be considered in a later document.

E-4.1 Steric relations at saturated bridgeheads common to two rings are denoted by *cis* or *trans*, followed by a hyphen and placed before the name of the ring system, according to the relative positions of the exocyclic atoms or groups attached to the bridgeheads. Such rings are said to be *cis*-fused or *trans*-fused.

Examples:



cis-Decalin

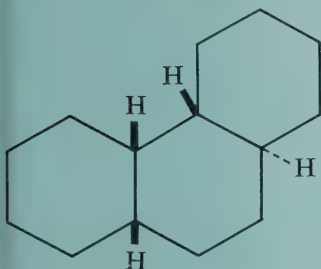


1-Methyl-*trans*-tricyclo[8.3.1.0^{3,8}]tetradeca-3(8),4,6-triene

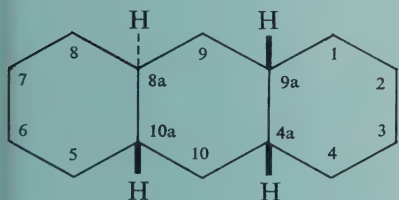
E-4.2 Steric relations at more than one pair of saturated bridgeheads in a polycyclic compound are denoted by *cis* or *trans*, each followed by a hyphen and, when necessary, the corresponding locant of the lower-numbered bridgehead and

a second hyphen, all placed before the name of the ring system. Steric relations between the nearest atoms^o of *cis*- or *trans*-bridgehead pairs may be described by affixes *cisoid* or *transoid*, followed by a hyphen and, when necessary, the corresponding locants and a second hyphen, the whole placed between the designations of the *cis*- or *trans*-ring junctions concerned. When a choice remains amongst nearest atoms, the pair containing the lower-numbered atom is selected. *cis* and *trans* are not abbreviated in such cases. In complex cases, however, designation may be more simply effected by the sequence rule procedure (see Appendix 2).

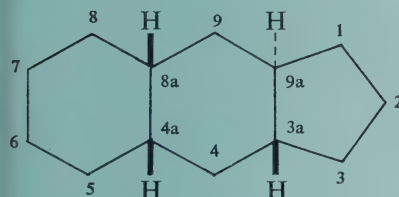
Examples:



cis-cisoid-trans-Perhydropheanthrene



cis-cisoid-4a,10a-trans-Perhydroacridine
or *rel*-(4a*S*,8a*S*,9a*S*,10a*R*)-Perhydroacridine^o



trans-3a-cisoid-3a,4a-cis-4a-Perhydro-
benz[*f*]indene
or *rel*-(3a*R*,4a*S*,8a*R*,9a*R*)-Perhydro-
benz[*f*]indene

E-5 Chirality

E-5.1 The property of non-identity of an object with its mirror image is termed chirality. An object, such as a molecule in a given configuration or conformation, is termed chiral when it is not identical with its mirror image; it is termed achiral when it is identical with its mirror image.

Notes: (1) Chirality is equivalent to handedness, the term being derived from the Greek *Χεῖρ* = hand.

(2) All chiral molecules are molecules of optically active compounds, and molecules of all optically active compounds are chiral. There is a 1:1 correspondence between chirality and optical activity.

The term "nearest atoms" denotes those linked together through the smallest number of atoms, irrespective of actual separation in space. For instance, in the second Example to this Rule, the atom 4a is "nearer" to 10a than to 8a.

^o For the designation *rel*- see Rule E-5.10.

- (3) In organic chemistry the discussion of chirality usually concerns the individual molecule or, more strictly, a model of the individual molecule. The chirality of an assembly of molecules may differ from that of the component molecules, as in a chiral quartz crystal or in an achiral crystal containing equal numbers of dextrorotatory and laevorotatory tartaric acid molecules.
- (4) The chirality of a molecule can be discussed only if the configuration or conformation of the molecule is specifically defined or is considered as defined by common usage. In such discussions structures are treated as if they were (at least temporarily) rigid. For instance, ethane is configurationally achiral although many of its conformations, such as (A), are chiral; in fact, a configuration of a mobile molecule is chiral only if all its possible conformations are chiral; and conformations of ethane such as (B) and (C) are achiral.



(A)

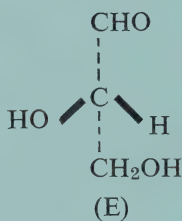
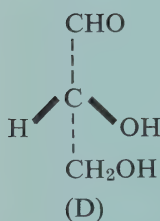


(B)

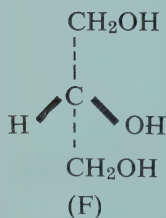


(C)

Examples:



(D) and (E) are mirror images and are not identical, not being superposable. They represent chiral molecules. They represent (D) dextro-rotatory and (E) laevorotatory glyceraldehyde.



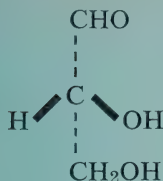
(F) is identical with its mirror image. It represents an achiral molecule, namely, a molecule of 1,2,3-propanetriol (glycerol).

E-5.2 The term asymmetry denotes absence of any symmetry. An object, such as a molecule in a given configuration or conformation, is termed asymmetric if it has no element of symmetry.

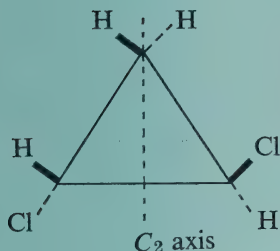
Notes: (1) All asymmetric molecules are chiral, and all compounds composed of them are therefore optically active; however, not all chiral molecules are asymmetric since some molecules having axes of rotation are chiral.

(2) Notes (3) and (4) to Rule E-5.1 apply also in discussions of asymmetry.

Examples:



has no element of symmetry and represents a molecule of an optically active compound.



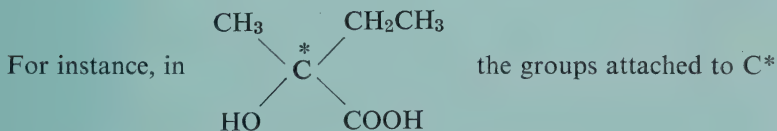
has a C_2 axis of rotation; it is chiral although not asymmetric, and is therefore a molecule of an optically active compound.

E-5.3 (a) An asymmetric atom is one that is tetrahedrally bonded to four different atoms or groups, none of the groups being the mirror image of any of the others.

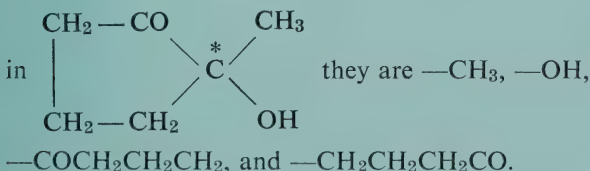
(b) An asymmetric atom may be said to be at a chiral centre since it lies at the centre of a chiral tetrahedral structure. In a general sense, the term “chiral centre” is not restricted to tetrahedral structures; the structure may, for instance, be based on an octahedron or tetragonal pyramid.

(c) When the atom by which a group is attached to the remainder of a molecule lies at a chiral centre the group may be termed a chiral group.

- Notes: (1) The term “asymmetric”, as applied to a carbon atom in rule E-5.3 (a), was chosen by van't Hoff because there is no plane of symmetry through a tetrahedron whose corners are occupied by four atoms or groups that differ in scalar properties. For differences of vector sense between the attached groups see Rule E-5.8.
- (2) In Sub-section E-5 the word “group” is used to denote the series of atoms attached to one bond.



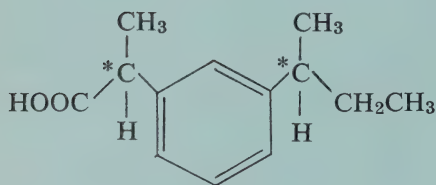
are $-\text{CH}_3$, $-\text{OH}$, $-\text{CH}_2\text{CH}_3$, and $-\text{COOH}$;



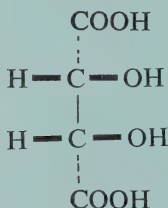
- (3) For the chiral axis and chiral plane (which are less common than the chiral centre) see Appendix 2.

- (4) There may be more than one chiral centre in a molecule and these centres may be identical, or structurally different, or structurally identical but of opposite chirality; however, presence of an equal number of structurally identical chiral groups of opposite chirality, and no other chiral group, leads to an achiral molecule. These statements apply also to chiral axes and chiral planes. Identification of the sites and natures of the various factors involved is essential if the overall chirality of a molecule is to be understood.
- (5) Although the term “chiral group” is convenient for use in discussions it should be remembered that chirality attaches to molecules and not to groups or atoms. For instance, although the *sec*-butyl group may be termed chiral in dextrorotatory 2-*sec*-butylnaphthalene, it is not chiral in the achiral compound $(\text{CH}_3\text{CH}_2)(\text{CH}_3)\text{CH}-\text{CH}_3$.

Examples:



In this chiral compound there are two asymmetric carbon atoms, marked C^* , each lying at a chiral centre. These atoms form part of different chiral groups, namely, $-\text{CH}(\text{CH}_3)\text{COOH}$ and $-\text{CH}(\text{CH}_3)\text{CH}_2\text{CH}_3$.



In this molecule (*meso*-tartaric acid) the two central carbon atoms are asymmetric atoms and each is part of a chiral group $-\text{CH}(\text{OH})\text{COOH}$. These groups, however, although structurally identical, are of opposite chirality, so that the molecule is achiral.

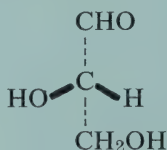
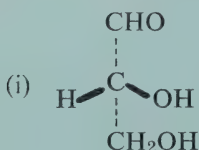
E-5.4 Molecules that are mirror images of one another are termed enantiomers and may be said to be enantiomeric. Chiral groups that are mirror images of one another are termed enantiomeric groups.

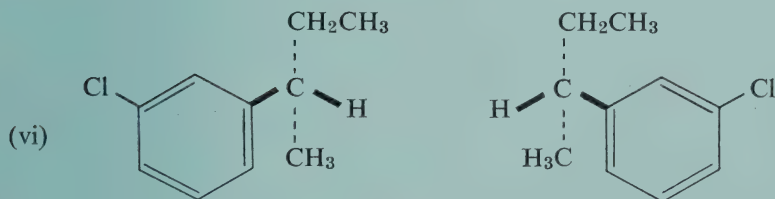
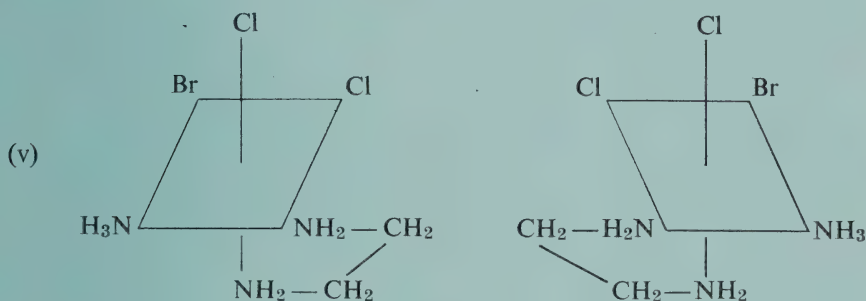
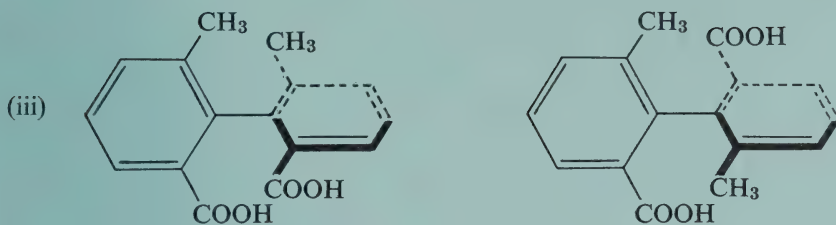
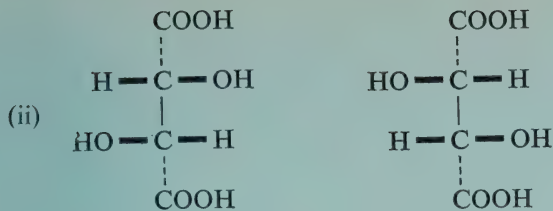
Hence: enantiomerism (phenomenological)

Note: Although the adjective enantiomeric may be applied to groups, enantiomerism strictly applies only to molecules (see Note (5) to Rule E-5.3).

Examples:

The following pairs of molecules are enantiomeric.





The *sec*-butyl groups in (vi) are enantiomeric.

E-5.5 When equal amounts of enantiomeric molecules are present together, the product is termed racemic, independently of whether it is crystalline, liquid, or gaseous. A homogeneous solid phase composed of equimolar amounts of enantiomeric molecules is termed a racemic compound. A mixture of equimolar amounts of enantiomeric molecules present as separate solid phases is termed a racemic mixture. Any homogeneous solid containing equimolar amounts of enantiomeric molecules is termed a racemate.

Examples:

The mixture of two kinds of crystal (mirror-image forms) that separate below 28°C from an aqueous solution containing equal amounts of dextrorotatory and laevorotatory sodium ammonium tartrate is a racemic mixture.

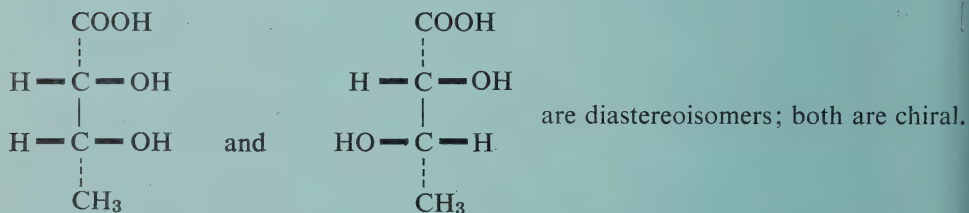
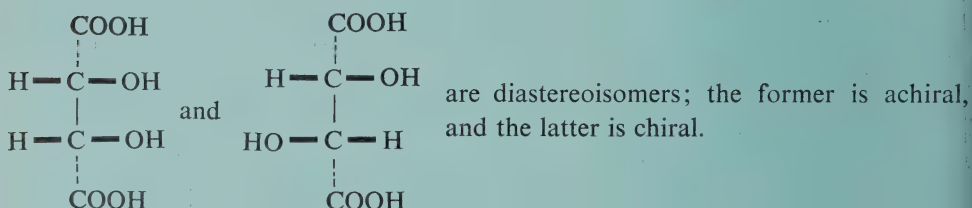
The symmetrical crystals that separate from such a solution above 28°C, each containing equal amounts of the two salts, provide a racemic compound.

E-5.6 Stereoisomers that are not enantiomeric are termed diastereoisomers.

Hence: diastereoisomeric (adjectival)
diastereoisomerism (phenomenological)

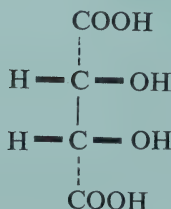
Note: Diastereoisomers may be chiral or achiral.

Examples:

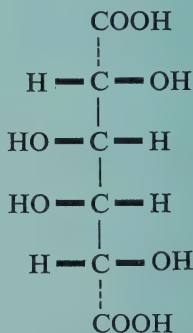


E-5.7 A compound whose individual molecules contain equal numbers of enantiomeric groups, identically linked, but no other chiral group, is termed a *meso*-compound.

Example:



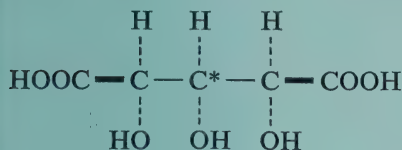
meso-Tartaric acid



Galactaric acid

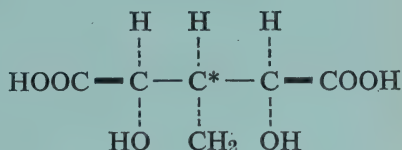
E-5.8 An atom is termed pseudoasymmetric when bonded tetrahedrally to one pair of enantiomeric groups (+)-a and (–)-a and also to two atoms or groups b and c that are different from group a, different from each other, and not enantiomeric with each other.

Examples:



(A)

C* are pseudoasymmetric



(B)

Notes: (1) The orientation, in space, of the atoms around a pseudoasymmetric atom is not reversed on reflexion; for a chiral atom (see Note to Rule E-5.3) this orientation is always reversed.

- (2) Molecules containing pseudoasymmetric atoms may be achiral or chiral. If ligands b and c are both achiral, the molecule is achiral as in the first example to this Rule. If either or both of the non-enantiomeric ligands b and c are chiral, the molecule is chiral, as in the second example to this Rule, that is the molecule is not identical with its mirror image. A

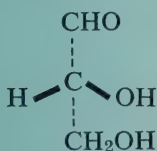
molecule $\begin{array}{c} (+)\text{-a} \diagdown \\ (-)\text{-a} \diagup \end{array} \text{X} \begin{array}{c} \text{---} \text{b} \\ \text{---} \text{c} \end{array}$ is also chiral if b and c are enantiomeric,

that is, if the molecule can be symbolized as $\begin{array}{c} (+)\text{-a} \diagdown \\ (-)\text{-a} \diagup \end{array} \text{X} \begin{array}{c} \text{---} \text{b-(+)} \\ \text{---} \text{b-(-)} \end{array}$, but then, by definition, it does not contain a pseudoasymmetric atom.

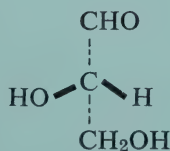
- (3) Compounds differing at a pseudoasymmetric atom belong to the larger class of diastereoisomers.
- (4) In example (A), interchange of H and OH on C* gives a different achiral compound, which is an achiral diastereoisomer of (A) (see Rule E-5.6). In example (B), diastereoisomers are produced by inversion at C* or ϕC , giving in all four diastereoisomers, all chiral because of the $-\text{CH}(\text{CH}_3)\text{CH}_2\text{CH}_3$ group.

E-5.9 Names of chiral compounds whose absolute configuration is known are differentiated by prefixes *R*, *S*, etc., assigned by the sequence-rule procedure (see Appendix 2), preceded when necessary by the appropriate locants.

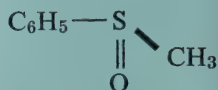
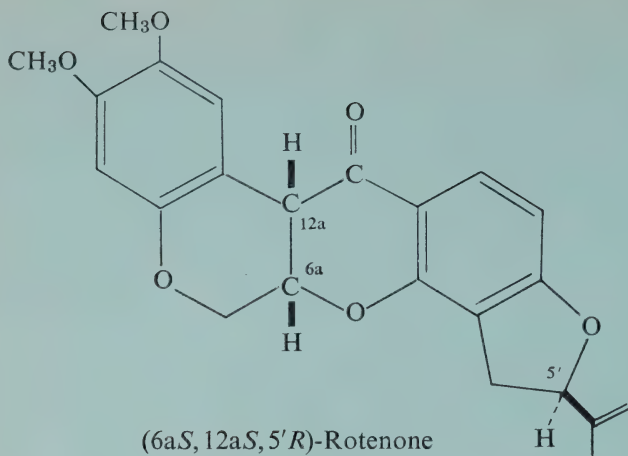
Examples:



(*R*)-Glyceraldehyde



(*S*)-Glyceraldehyde



Methyl phenyl
(*R*)-sulfoxide

E-5.10 (a) Names of compounds containing chiral centres, of which the relative but not the absolute configuration is known, are differentiated by prefixes *R*^{*}, *S*^{*} (spoken *R* star, *S* star), preceded when necessary by the appropriate locants, these prefixes being assigned by the sequence-rule procedure (see Appendix 2) on the arbitrary assumption that the prefix first cited is *R*.

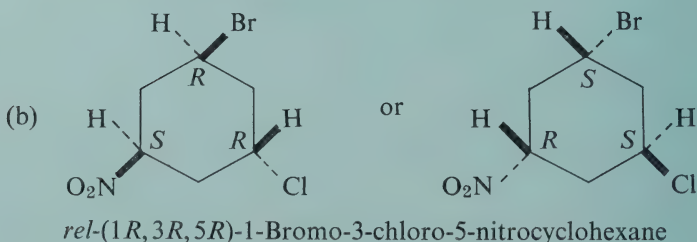
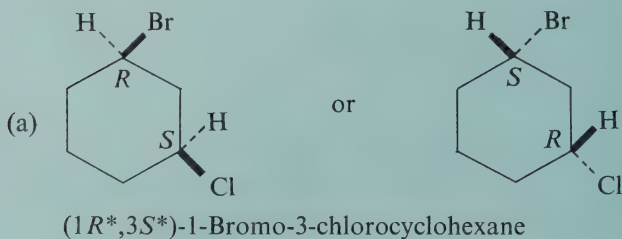
(b) In complex cases the stars may be omitted and, instead, the whole name is prefixed by *rel*- (for *relative*).

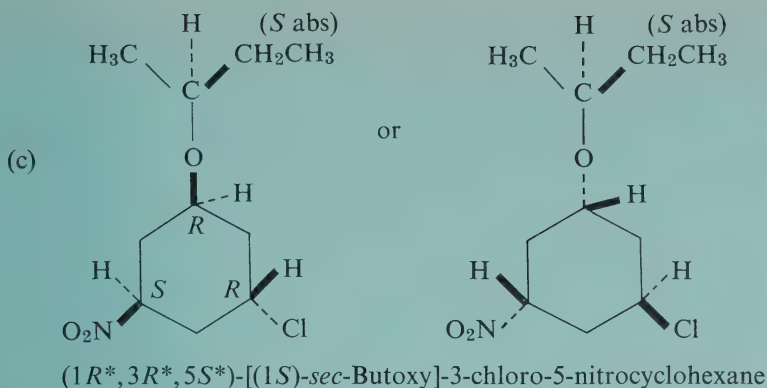
(c) When only relative configuration is known, enantiomers are distinguished by a prefix (+)- or (−)-, referring to the direction of rotation of plane-polarized light passing through them (wavelength, temperature, solvent, and/or concentration should also be specified, particularly when known to affect the sign).

(d) When a substituent of known absolute chirality is introduced into a compound of which only the relative configuration is known, then starred symbols *R*^{*}, *S*^{*} are used and not the prefix *rel*-.

Note: This Rule does not form part of the procedure formulated in the sequence-rule papers by CAHN, INGOLD, and PRELOG (see Appendix 2).

Examples:





E-5.11 When it is desired to express relative or absolute configuration with respect to a class of compound, specialized local systems may be used. The sequence rule may, however, be used additionally for positions not amenable to treatment by the local system.

Examples:

gluco, *arabino*, etc., combined when necessary with D or L, for carbohydrates and their derivatives (see IUPAC/IUB Tentative Rules for Carbohydrate Nomenclature, in the press).

D, L for amino acids and peptides (see Comptes rendus of the 16th IUPAC Conference, New York, 1951, pp. 107–108).

D, L and a series of other prefixes and trivial names for cyclitols and their derivatives (see IUPAC/IUB Tentative Rules for the Nomenclature of Cyclitols, 1967, IUPAC Information Bulletin, No. 32 (August 1968, pp. 51–80).

α , β , and a series of trivial names for steroids and related compounds (see IUPAC/IUB Revised Tentative Rules for the Nomenclature of Steroids, 1967, in the press).

The α , β system for steroids can be extended to other classes of compound such as terpenes and alkaloids when their absolute configurations are known; it can also be combined with stars or the use of a prefix *rel*- when only the relative configurations are known.

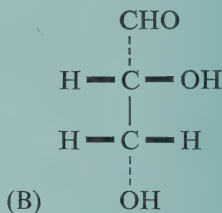
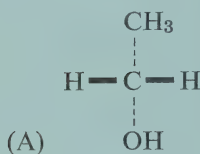
In spite of the Rules of Subsection E-2, *cis* and *trans* are used when the arrangement of the atoms constituting an unsaturated backbone is the most important factor, as, for instance, in polymer chemistry and for carotenoids. When a series of double bonds of the same stereochemistry occurs in a backbone, the prefix *all-cis* or *all-trans* may be used.

E-5.12 (a) An achiral object having at least one pair of features that can be distinguished only by reference to a chiral object or to a chiral reference frame is said to be prochiral, and the property of having such a pair of features is termed prochirality. A consequence is that if one of the paired features of a prochiral object is considered to differ from the other the resultant object is chiral.

(b) In a molecule an achiral centre or atom is said to be prochiral if it would be held to be chiral when two attached atoms or groups, that taken in isolation are indistinguishable, are considered to differ.

- Notes: (1) For a tetrahedrally bonded atom this requires a structure $Xaabc$ (where none of the groups a , b , or c is the enantiomer of another).
 (2) For a fuller exploration of this concept, which is of particular importance to biochemists and spectroscopists, and for its extension to axes, planes, and unsaturated compounds, see K. R. HANSON, *J. Amer. Chem. Soc.*, 88, 2731 (1966).

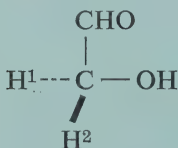
Examples:



In both examples (A) and (B) the methylene carbon atom is prochiral; in both cases it would be held to be at a chiral centre if one of the methylene hydrogen atoms were considered to differ from the other. An actual replacement of one of these protium atoms by, say, deuterium would produce an actual chiral centre at the methylene carbon atom; as a result compound (A) would become chiral, and compound (B) would be converted into one of two diastereoisomers.

E-5.13 Of the identical pair of atoms or groups in a prochiral compound, that one which leads to an (*R*)-compound when considered to be preferred to the other by the sequence rule (without change in priority with respect to other ligands) is termed *pro-R*, and the other is termed *pro-S*.

Example:

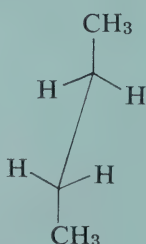
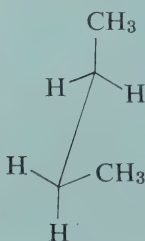


H^1 is *pro-R*. H^2 is *pro-S*.

E-6 Conformations

E-6.1 A molecule in a conformation into which its atoms return spontaneously after small displacements is termed a conformer.

Examples:



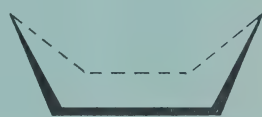
are different conformers.

E-6.2 (a) When, in a six-membered saturated ring compound, atoms in relative positions 1, 2, 4, and 5 lie in one plane, the molecule is described as in the chair or boat conformation according as the other two atoms lie, respectively, on opposite sides or on the same side of that plane.

Examples:



Chair



Boat

Note: These and similar representations are idealized, minor divergences being neglected.

(b) A molecule of a monounsaturated six-membered ring compound is described as being in the half-chair or half-boat conformation according as the atoms not directly bound to the doubly bonded atoms lie, respectively, on opposite sides or on the same side of the plane containing the other four (adjacent) atoms.

Examples:



Half-chair



Half-boat

(c) A median conformation through which one boat form passes during conversion into the other boat form is termed a twist conformation. Similar twist conformations are involved in conversion of a chair into a boat form or *vice versa*.

Example:



Boat

Twist

Boat

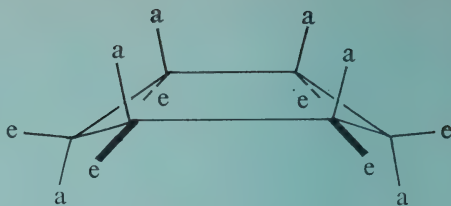
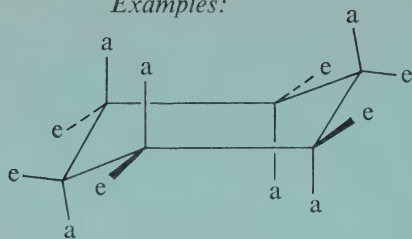
E-6.3 (a) Bonds to a tetrahedral atom in a six-membered ring are termed equatorial or axial according as they or their projections make a small or a large angle, respectively, with the plane containing a majority of the ring atoms. Atoms or groups attached to such bonds are also said to be equatorial or axial, respectively.

Notes: (1) See, however, pseudo-equatorial and pseudo-axial [Rule 6.3(b)].

(2) The terms equatorial and axial may be abbreviated to *e* and *a* when attached to formulae; these abbreviations may also be used in names of compounds and are there placed in parentheses after the appropriate locants, for example, 1(*e*)bromo-4(*a*)-chlorocyclohexane.

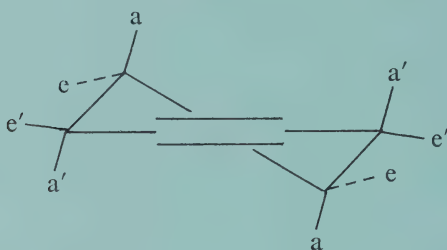
⚠ The terms axial, equatorial, pseudo-axial, and pseudo-equatorial [see Rule E-6.3(b)] may be used also in connexion with other than six-membered rings if, but only if, their interpretation is then still beyond dispute.

Examples:



(b) Bonds from atoms directly attached to the doubly bonded atoms in a mono-unsaturated six-membered ring are termed pseudo-equatorial or pseudo-axial according as the angles that they make with the plane containing the majority of the ring atoms approximate to those made by, respectively, equatorial or axial bonds from a saturated six-membered ring. Pseudo-equatorial and pseudo-axial may be abbreviated to e' and a' , respectively, when attached to formulae; these abbreviations may also be used in names, then being placed in parentheses after the appropriate locants.

Example:

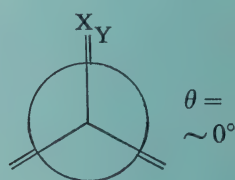
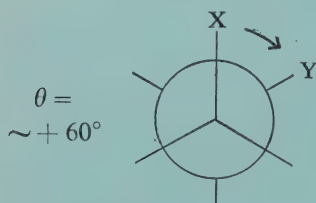


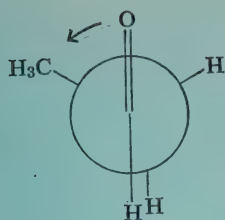
E-6.4 Torsion angle: In an assembly of attached atoms X-A-B-Y, where neither X nor Y is collinear with A and B, the smaller angle subtended by the bonds X-A and Y-B in a plane projection obtained by viewing the assembly along the axis A-B is termed the torsion angle (denoted by the Greek lower-case letter theta θ or omega ω). The torsion angle is considered positive or negative according as the bond to the front atom X or Y requires to be rotated to the right or left, respectively, in order that its direction may coincide with that of the bond to the rear selected atom Y or X. The multiplicity of the bonding of the various atoms is irrelevant. A torsion angle also exists if the axis for rotation is formed by a collinear set of more than two atoms directly attached to each other.

Notes: (1) It is immaterial whether the projection be viewed from the front or the rear.
(2) For the use of torsion angles in describing molecules see Rule E-6.6

Examples

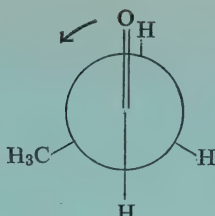
(For construction of Newman projections, as here, see Rule E-7.2):





Newman projections of
propionaldehyde

$$\theta = \sim -60^\circ$$



$$\theta = \sim -120^\circ$$

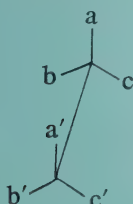


Newman projection of
hydrogen peroxide

$$\theta = \sim 180^\circ$$

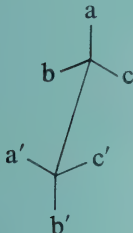
E-6.5 If two atoms or groups attached at opposite ends of a bond appear one directly behind the other when the molecule is viewed along this bond, these atoms or groups are described as eclipsed, and that portion of the molecule is described as being in the eclipsed conformation. If not eclipsed, the atoms or groups and the conformation may be described as staggered.

Examples:



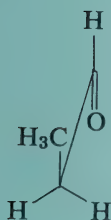
Eclipsed conformation.

The pairs a/a', b/b', and c/c' are eclipsed.



Staggered conformation.

All the attached groups are staggered.



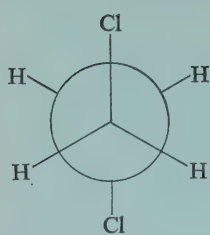
Projection of $\text{CH}_3\text{CH}_2\text{CHO}$.

The CH_3 and the H of the CHO are eclipsed.

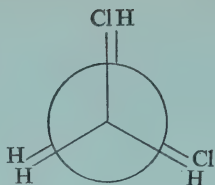
The O and the H's of CH_2 in CH_2CH_3 are staggered.

E-6.6 Conformations are described as synperiplanar (*sp*), synclinal (*sc*), anti-clinal (*ac*), or antiperiplanar (*ap*) according as the torsion angle is within $\pm 30^\circ$ of 0° , $\pm 60^\circ$, $\pm 120^\circ$, or $\pm 180^\circ$, respectively; the letters in parentheses are the corresponding abbreviations. Atoms or groups are selected from each set to define the torsion angle according to the following criteria: (1) if all the atoms or groups of a set are different, that one of each set that is preferred by the sequence rule; (2) if one of a set is unique, that one; or (3) if all of a set are identical, that one which provides the smallest torsion angle.

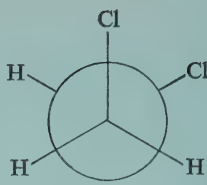
Examples:



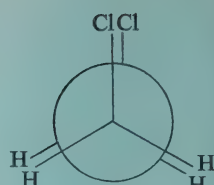
antiperiplanar



anticlinal

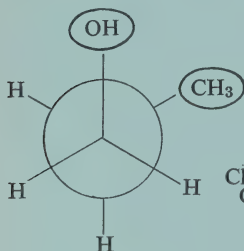


synclinal

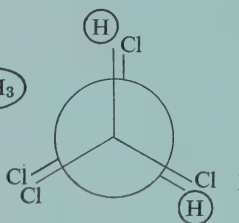


synperiplanar

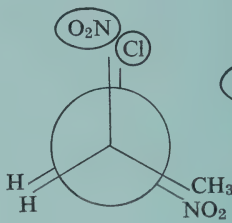
In the above conformations, all $\text{CH}_2\text{Cl}-\text{CH}_2\text{Cl}$, the two Cl atoms decide the torsion angle.



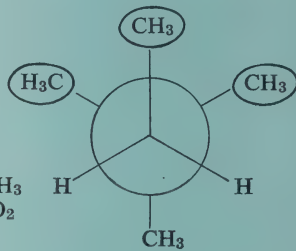
synclinal



anticlinal



synperiplanar



synclinal

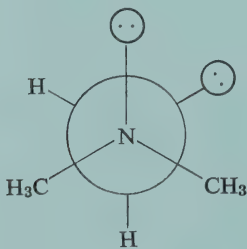
Criterion for:

rear atom 2
front atom 2

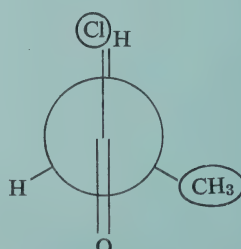
2
2

1
1

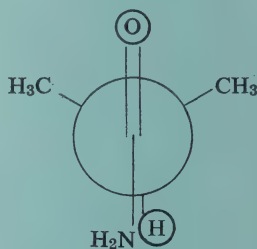
3
2



$(\text{CH}_3)_2\text{N}-\text{NH}_2$
synclinal^o



$\text{CH}_3\text{CH}_2-\text{COCl}$
anticlinal



$(\text{CH}_3)_2\text{CH}-\text{CONH}_2$
antiperiplanar

Criterion for:

rear atom 2
front atom 2

2
1

2
1

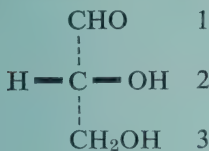
E-7 Stereoformulae

E-7.1 In a Fischer projection the atoms or groups attached to a tetrahedral centre are projected on to the plane of the paper from such an orientation that atoms or groups appearing above or below the central atom lie behind the plane of the

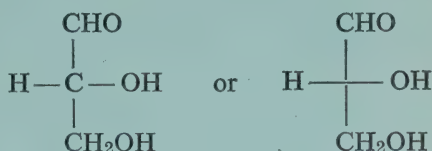
◊ The lone pair of electrons (represented by two dots) on the nitrogen atoms are the unique substituents that decide the description of the conformation (these are the "phantom atoms" of the sequence-rule symbolism).

paper and those appearing to left and right of the central atom lie in front of the plane of the paper, and that the principal chain appears vertical with the lowest-numbered chain member at the top.

Example:



Orientation

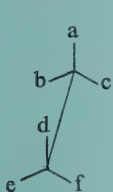


Fischer projection

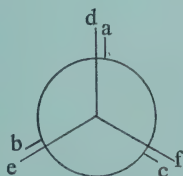
- Notes:* (1) The first of the two types of Fischer projection should be used whenever convenient.
- (2) If a Fischer projection formula is rotated through 180° in the plane of the paper, the upward and downward bonds from the central atom still project behind the plane of the paper, and the sideways bonds project in front of that plane. If, however, the formula is rotated through 90° in the plane of the paper, the upward and downward bonds now project in front of the plane of the paper and the sideways bonds project behind that plane.

E-7.2 To prepare a Newman projection a molecule is viewed along the bond between two atoms; a circle is used to represent these atoms, with lines from outside the circle towards its centre to represent bonds to other atoms; the lines that represent bonds to the nearer and the further atom end at, respectively, the centre and the circumference of the circle. When two such bonds would be coincident in the projection, they are drawn at a small angle to each other.

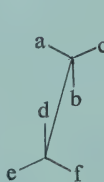
Examples:



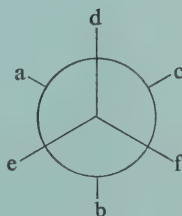
Perspective



Newman projection



Perspective



Newman
projection

E-7.3 General note

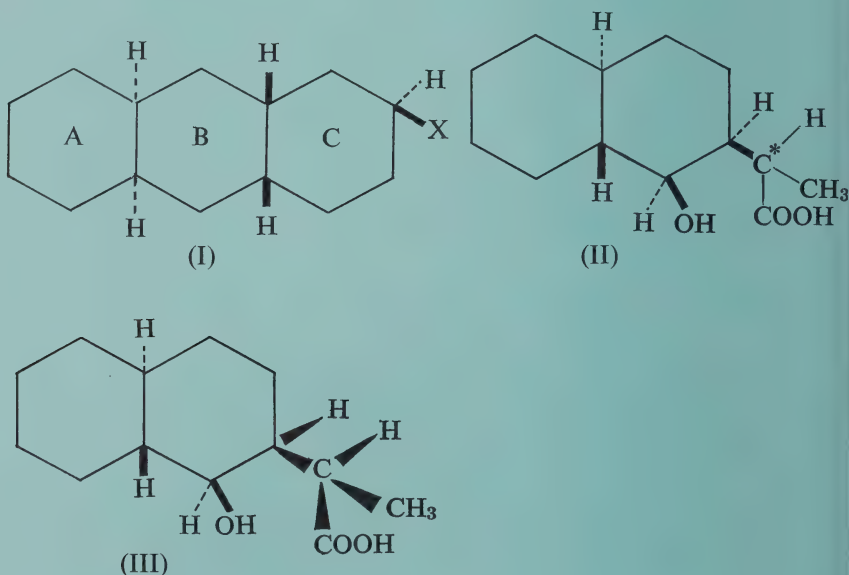
Formulae that display stereochemistry should be prepared with extra care so as to be unambiguous and, whenever possible, self-explanatory. It is inadvisable to try to lay down rules that will cover every case, but the following points should be borne in mind.

♦ Cf. M.S. NEWMAN: *Chem. Progr. Kreskge-Hooker Sci. Lab. Rep.* 13, 111 (1952); *J. Chem. Educ.* 33, 344 (1955); "Steric Effects in Organic Chemistry", John Wiley & Sons Inc., New York 1956, p.6).

A thickened line (—) denotes a bond projecting from the plane of the paper towards an observer, a broken line (- -) denotes a bond projecting away from an observer, and, when this convention is used, a full line of normal thickness (—) denotes a bond lying in the plane of the paper. A wavy line (~~~~) may be used to denote a bond whose direction cannot be specified or, if it is explained in the text, a bond whose direction it is not desired to specify in the formula. Dotted lines (.....) should preferably not be used to denote stereochemistry, and never when they are used in the same paper to denote mesomerism, intermediate states, etc. Wedges should not be used as complement to broken lines (but see below). Single large dots have sometimes been used to denote atoms or groups attached at bridgehead positions and lying above the plane of the paper, with open circles to denote them lying below the plane of the paper, but this practice is strongly deprecated.

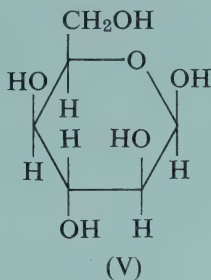
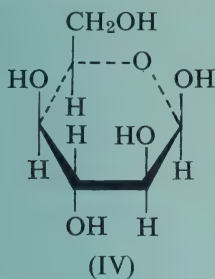
Hydrogen or other atoms or groups attached at sterically designated positions should never be omitted.

In chemical formulae, rings are usually drawn with lines of normal thickness, that is, as if they lay wholly in the plane of the paper even though this may be known not to be the case. In a formula such as (I) it is then clear that the H atoms attached at the A/B ring junction lie further from the observer than these bridgehead atoms, that the H atoms attached at the B/C ring junction lie nearer to the observer than those bridgehead atoms, and that X lies nearer to the observer than the neighbouring atom of ring C.

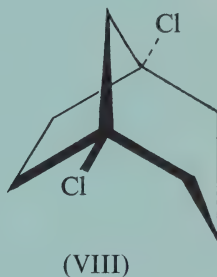
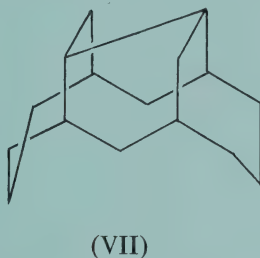
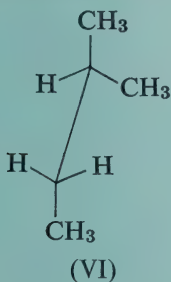


However, ambiguity can then sometimes arise, particularly when it is necessary to show stereochemistry within a group such as X attached to the rings that are drawn planar. For instance, in formula (II), the atoms O and C*, lying above the plane of the paper, are attached to ring B by thick bonds; but then, when showing the stereochemistry at C*, one finds that the bond *from* C* to ring B projects away from the observer and so should be a broken line. Such difficulties can be overcome by using wedges in place of lines, the broader end of the wedge being considered nearer to the observer, as in (III).

In some fields, notably for carbohydrates, rings are conveniently drawn as if they lay perpendicular to the plane of the paper, as represented in (IV); however, conventional formulae such as (V), with the lower bonds considered as the nearer to the observer, are so well established that it is rarely necessary to elaborate this to form (IV).



By a similar convention, in drawings such as (VI) and (VII), the lower sets of bonds are considered to be nearer than the upper to the observer. In (VII), note the gaps in the rear lines to indicate that the bonds crossing them pass in front (and thus obscure sections of the rear bonds). In some cases, when atoms have to be shown as lying in several planes, the various conventions may be combined, as in (VIII).



In all cases the overriding aim should be clarity.

APPENDIX 1

Configuration and Conformation

See Rules E-1.4 and E-1.5.

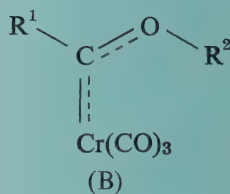
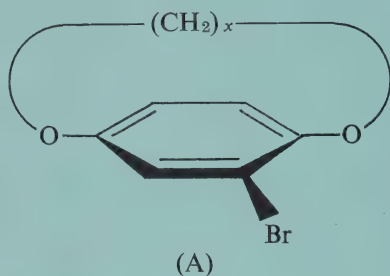
Various definitions have been propounded to differentiate configurations from conformations.

The original usage was to consider as conformations those arrangements of the atoms of a molecule in space that can be interconverted by rotation(s) around a single bond, and as configurations those other arrangements whose interconversion by rotation requires bonds to be broken and then re-formed differently. Interconversion of different configurations will then be associated with substantial energies of activation, and the various species will be separable; but interconversion of different conformations will normally be associated with less activation energy, and the various species, if separable, will normally be more readily interconvertible. These differences in activation energy and stability are often large.

Nevertheless, rigid differentiation on such grounds meets formidable difficulties. Differentiation by energy criteria would require an arbitrary cut in a continuous

series of values. Differentiation by stability of isolated species requires arbitrary assumptions about conditions and half-lives. Differentiation on the basis of rotation around single bonds meets difficulties connected both with the concept of rotation and with the selection of single bonds as requisites; and these need more detailed discussion here.

Enantiomeric biaryls are nowadays usually considered to differ in conformation, any difficulty in rotation about the 1,1'-bond due to steric hindrance between the neighbouring groups being considered to be overcome by bond bending and/or bond stretching, even though the movements required must closely approach bond breaking if these substituents are very large. Similar doubts about the possibility of rotation occur with a molecule such as (A), where rotation of the benzene ring around the oxygen-to-ring single bonds affords easy interconversion if x is large but appears to be physically impossible if x is small; and no critical size of x can be reasonably established. For reasons such as this, Rules E-1.4 and E-1.5 are so worded as to be independent of whether rotation appears physically feasible or not (see Note 2 to those Rules).



The second difficulty arises in the many cases where rotation is around a bond of fractional order between one and two, as in the helicenes, crowded aromatic molecules, metallocenes, amides, thioamides, and carbene-metal coordination compounds (such as B). The term conformation is customarily used in these cases and that appears a reasonable extension of the original conception, though it will be wise to specify the usage if the reader might be in doubt.

When interpreted in these ways, Rules E-1.4 and E-1.5 reflect the most frequent usage of the present day and provide clear distinctions in most situations.

Nevertheless, difficulties remain and a number of other usages have been introduced.

It appears to some workers that, once it is admitted that change of conformation may involve rotation about bonds of fractional order between one and two, it is then illogical to exclude rotation about classical double bonds because interconversion of open-chain *cis-trans*-isomers depends on no fundamentally new principle and is often relatively easy, as for certain alkene derivatives such as stilbenes and for azo compounds, by irradiation. This extension is indeed not excluded by Rules E-1.4 and E-1.5, but if it is applied that fact should be explicitly stated.

A further interpretation is to regard a stereoisomer possessing some degree of stability (that is, one associated with an energy hollow, however shallow) as a configurational isomer, the other arrangements in space being termed conformational isomers; the term conformer (Rule E-6.1) is then superfluous. This definition, however, requires a knowledge of stability (energy relations) that is not always available.

In another view a configurational isomer is any stereoisomer that can be isolated or (for some workers) whose existence can be established (for example, by physical methods); all other arrangements then represent conformational isomers. But it is then impossible to differentiate configuration from conformation without involving experimental efficiency or conditions of observation.

Yet another definition is to regard a conformation as a precise description of a configuration in terms of bond distances, bond angles, and dihedral angles.

In none of the above views except the last is attention paid to extension or contraction of the bond to an atom that is attached to only one other atom, such as —H or =O . Yet such changes in interatomic distance due to non-bonded interactions may be important, for instance in hydrogen bonding, in differences due to crystal form, in association in solution, and in transition states. This area may repay further consideration.

Owing to the circumstances outlined above, the Rules E-1.4 and E-1.5 have been deliberately made imprecise, so as to permit some alternative interpretations; but they are not compatible with all the definitions mentioned above. The time does not seem ripe to legislate for other than the commoner usages or to choose finally between these.

It is, however, encouraging that no definition in this field has (yet) involved atomic vibrations for which, in all cases, only time-average positions are considered.

Finally it should be noted that an important school of thought uses conformation with the connotation of “a particular geometry of the molecule, *i.e.*, a description of atoms in space in terms of bond distances, bond angles, and dihedral angles”, a definition much wider than any discussed above.

APPENDIX 2

Outline of the Sequence Rule Procedure

The sequence rule procedure is a method of specifying the absolute molecular chirality (handedness) of a compound, that is, a method of specifying in which of two enantiomeric forms each chiral element of a molecule exists. For each chiral element in the molecule it provides a symbol, usually *R* or *S*, which is independent of nomenclature and numbering. These symbols define the chirality of the specific compound considered; they may not be the same for a compound and some of its derivatives; and they are not necessarily constant for chemically similar situations within a chemical or a biogenetic class. The procedure is applied directly to a three-dimensional model of the structure, and not to any two-dimensional projection thereof.

The method has been developed to cover all compounds with ligancy up to 4 and with ligancy 6 $\frac{1}{2}$, and for all configurations and conformations of such compounds. The following is an outline confined to the most common situations; it is essential to study the original papers, especially the 1966 paper⁴⁶, before using the sequence rule for other than fairly simple cases.

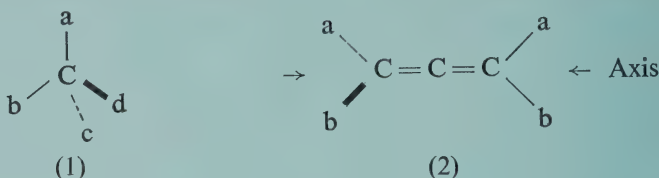
♦ Ligancy refers to the number of bonds from an atom, independently of the nature of the bonds.

♦♦ R.S. CAHN, (Sir) CHRISTOPHER INGOLD, V. PRELOG: *Angew. Chem. intern. Edit.* 5, 385 (1966) (in English); errata, *ibid.*, p. 511; *Angew. Chem.* 78, 413 (1966) (in German). Earlier papers: R.S. CAHN, C.K. INGOLD: *J. Chem. Soc. (London)* 1951, 612; R.S. CAHN, (Sir) CHRISTOPHER INGOLD, V. PRELOG: *Experientia* 12, 81 (1956). For a partial, simplified account see R.S. CAHN: *J. Chem. Educ.* 41, 116 (1964).

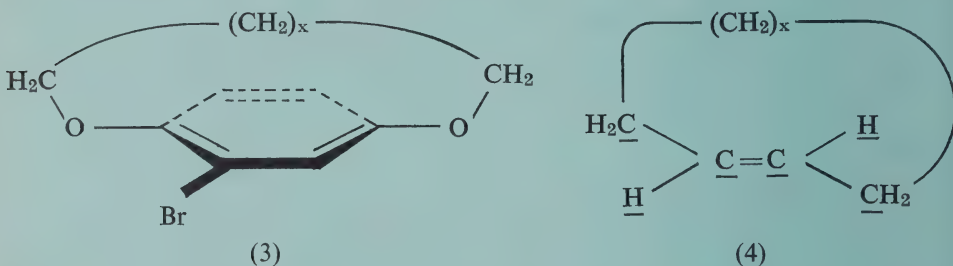
General basis

The sequence rule itself is a method of arranging atoms or groups (including chains and rings) in an order of precedence, often referred to as an order of preference; for discussion this order can conveniently be generalized as $a > b > c > d$, where $>$ denotes "is preferred to".

The first step, however, in considering a model is to identify the nature and position of each chiral element that it contains. There are three types of chiral element, namely, the chiral centre, the chiral axis, and the chiral plane. The chiral centre, which is very much the most commonly met, is exemplified by an asymmetric carbon atom with the tetrahedral arrangement of ligands, as in (1). A chiral axis is present in, for instance,



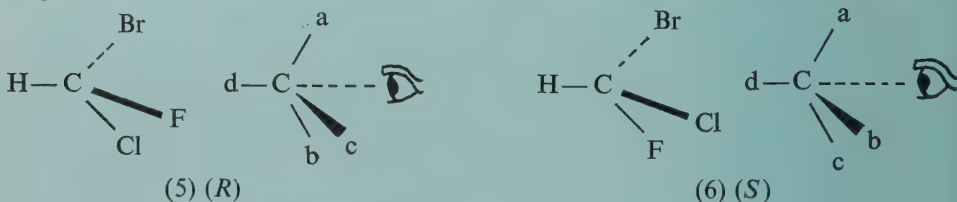
the chiral allenes such as (2) or the chiral biaryl derivatives. A chiral plane is exemplified by the plane containing the benzene ring and the bromine and oxygen atoms in the chiral compound (3), or by the underlined atoms in the cycloalkene (4). Clearly,



more than one type of chiral element may be present in one compound; for instance, group "a" in (2) might be a *sec*-butyl group which contains a chiral centre.

The chiral centre

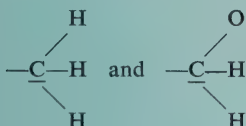
Let us consider first the simplest case, namely, a chiral centre (such as carbon) with four ligands, a, b, c, d which are all different atoms, tetrahedrally arranged, as in CHFCIBr. The four ligands are arranged in order of preference by means of the sequence rule; this contains five sub-rules, which are applied in succession so far as necessary to obtain a decision. The first sub-rule is all that is required in a great majority of actual cases; it states that ligands are arranged in order of decreasing atomic number, in the above case (a) Br > (b) Cl > (c) F > (d) H. There would be two (enantiomeric) forms of the compound and we can write these as (5) and (6). In the



sequence-rule procedure the model is viewed from the side remote from the least-preferred ligand (d), as illustrated. Then, tracing a path from a to b to c in (5) gives a clockwise course, which is symbolized by (*R*) (Latin *rectus*, right; for right-hand); in (6) it gives an anticlockwise course, symbolized as (*S*) (Latin *sinister*, left). Thus (5) would be named (*R*)-bromochlorofluoromethane, and (6) would be named (*S*)-bromochlorofluoromethane. Here already it may be noted that converting one enantiomer into another changes each *R* to *S*, and each *S* to *R*, always. It will be seen also that the chirality prefix is the same whether the alphabetical order is used, as above, for naming the substituents or whether this is done by the order of complexity (giving fluorochlorobromomethane).

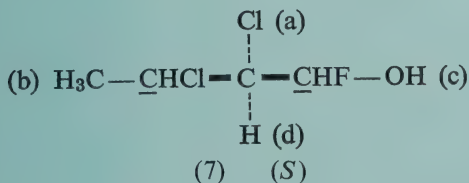
Next, suppose we have $\text{H}_3\text{C}-\text{CHClF}$. We deal first with the atoms directly attached to the chiral centre; so the four ligands to be considered are $\text{Cl} > \text{F} > \text{C}(\text{of CH}_3) > \text{H}$. Here the H's of the CH_3 are not concerned, because we do not need them in order to assign our symbol.

However, atoms directly attached to a centre are often identical, as for example the underlined C's in $\text{H}_3\text{C}-\text{CHCl}-\text{CH}_2\text{OH}$. For such a compound we at once establish a preference (a) $\text{Cl} > (\text{b,c}) \text{C}, \text{C} > (\text{d}) \text{H}$. Then to decide between the two C's we work outwards, to the atoms to which they in turn are directly attached and we then find

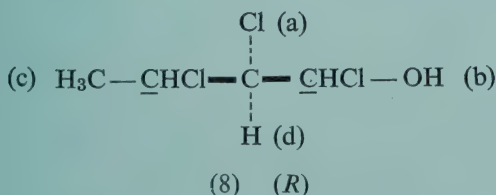


which we can conveniently write as $\text{C}(\text{H},\text{H},\text{H})$ and $\text{C}(\text{O},\text{H},\text{H})$. We have to compare $\text{H},\text{H},\text{H}$ with $\text{O},\text{H},\text{H}$, and since oxygen has a higher atomic number than hydrogen we have $\text{O} > \text{H}$ and thence the complete order $\text{Cl} > \text{C}(\text{of CH}_2\text{OH}) > \text{C}(\text{of CH}_3) > \text{H}$, so that the chirality symbol can then be determined from the three-dimensional model.

We must next meet the first complication. Suppose that we have a molecule (7):

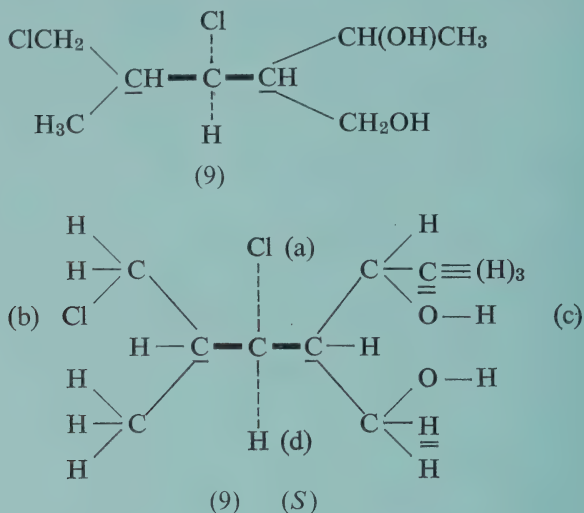


To decide between the two C's we first arrange the atoms attached to them in *their* order of preference, which gives C(Cl,C,H) on the left and C(F,O,H) on the right. Then we compare the preferred atom of one set (namely, Cl) with the preferred atom (F) of the other set; and as $\text{Cl} > \text{F}$ we arrive at the preferences $\text{a} > \text{b} > \text{c} > \text{d}$ shown in (7) and chirality (*S*). If, however, we had a compound (8):



we should have met $\underline{\text{C}}(\text{Cl}, \text{C}, \text{H})$ and $\underline{\text{C}}(\text{Cl}, \text{O}, \text{H})$ and, since the atoms of first preference are identical (Cl) we should have had to make the comparisons with the atoms of second preference, namely, $\text{O} > \text{C}$, which leads to the different chirality (*R*) as shown in (8).

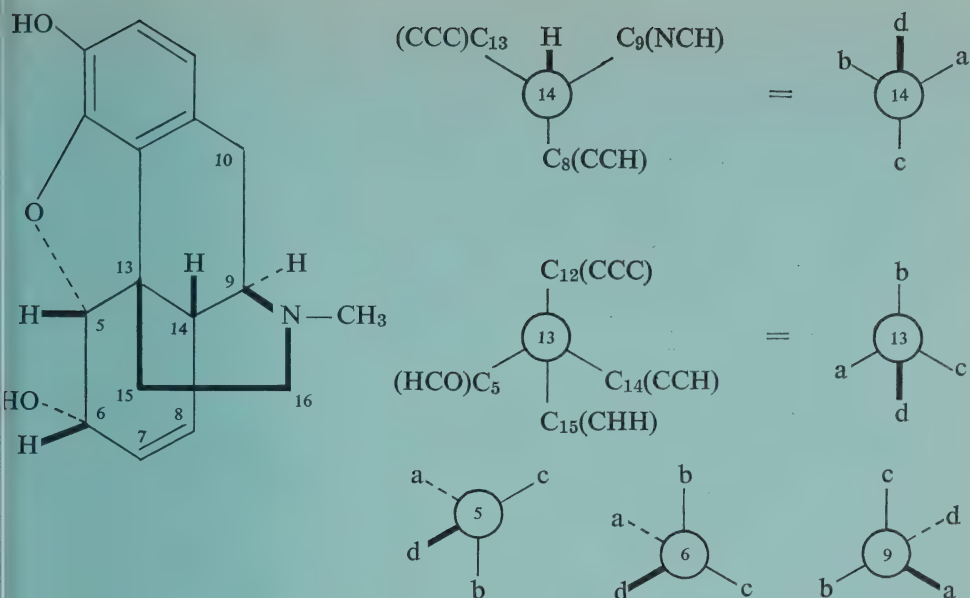
Branched ligands are treated similarly. Setting them out in full gives a picture that at first sight looks complex but the treatment is in fact simple. For instance, in compound (9) a first quick glance again shows (a) $\text{Cl} > (\text{b}, \text{c}) \underline{\text{C}}, \underline{\text{C}} > (\text{d}) \text{H}$.



When we expand the two $\underline{\text{C}}$'s we find they are both $\underline{\text{C}}(\text{C}, \text{C}, \text{H})$, so we continue exploration. Considering first the left-hand ligand we arrange the branches and their sets of atoms in order thus: $\text{C}(\text{Cl}, \text{H}, \text{H}) > \text{C}(\text{H}, \text{H}, \text{H})$; and on the right-hand side we have $\text{C}(\text{O}, \underline{\text{C}}, \text{H}) > \text{C}(\text{O}, \underline{\text{H}}, \text{H})$ (because $\underline{\text{C}} > \underline{\text{H}}$). We compare first the preferred of these branches from each side and we find $\text{C}(\text{Cl}, \text{H}, \text{H}) > \text{C}(\text{O}, \text{C}, \text{H})$ because $\text{Cl} > \text{O}$, and that gives the left-hand branch preference over the right-hand branch. That is all we need to do to establish chirality (*S*) for this highly branched compound (9). Note that it is immaterial here that, for the lower branches, the right-hand $\text{C}(\text{O}, \text{H}, \text{H})$ would have been preferred to the left-hand $\text{C}(\text{H}, \text{H}, \text{H})$; we did not need to reach that point in our comparisons and so we are not concerned with it; but we should have reached it if the two top (preferred) branches had both been the same CH_2Cl .

Rings, when met during outward exploration, are treated in the same way as branched chains.

With these simple procedures alone, quite complex structures can be handled; for instance, the analysis alongside formula (10) for natural morphine explains why the specification is as shown. The reason for considering C-12 as $\text{C}(\text{CCC})$ is set out in the next paragraphs.

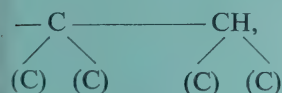


(10) (5*R*, 6*S*, 9*R*, 13*S*, 14*R*)-Morphine

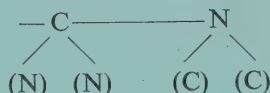
Now, using the sequence rule depends on exploring along bonds. To avoid theoretical arguments about the nature of bonds, simple classical forms are used. Double and triple bonds are split into two and three bonds, respectively. A $>\text{C}=\text{O}$ group is treated as $>\text{C}-\text{O}$, where the (O) and the (C) are duplicate representations of the



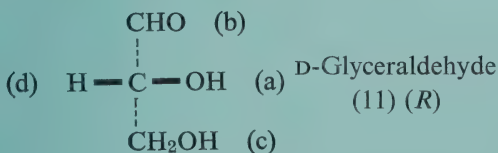
atoms at the other end of the double bond. $-\text{C}\equiv\text{CH}$ is treated as



and $-\text{C}\equiv\text{N}$ is treated as

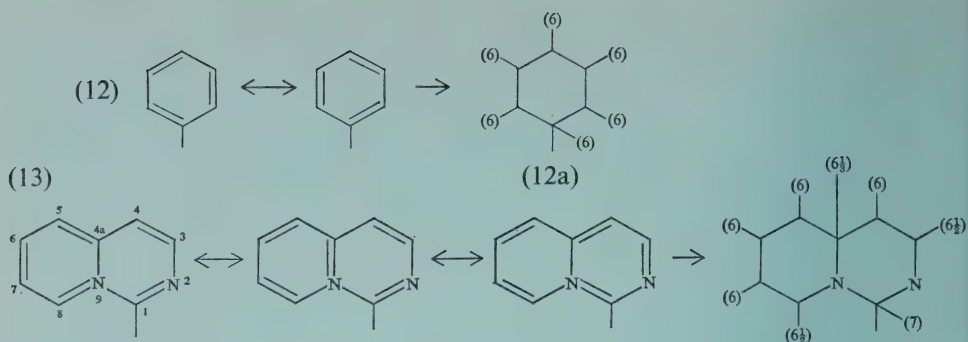


Thus in D-glyceraldehyde (11) the CHO group is treated as C(O,(O),H) and is thus preferred to the C(O,H,H) of the CH₂OH group, so that the chirality symbol is (*R*).



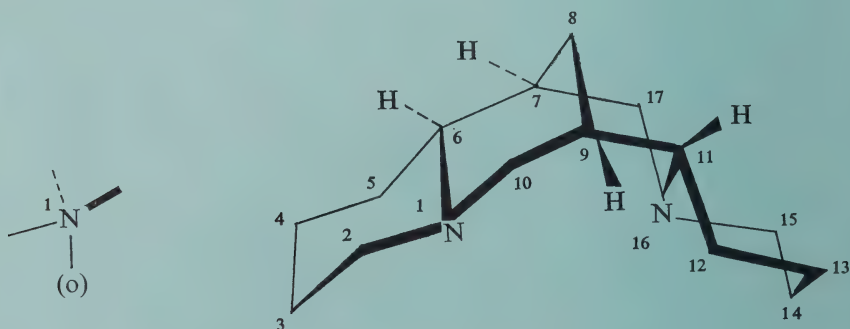
Only the doubly bonded atoms themselves are duplicated, and not the atoms or groups attached to them; the duplicated atoms may thus be considered as carrying three phantom atoms (see below) of atomic number zero. This may be important in deciding preferences in certain complicated cases.

Aromatic rings are treated as Kekulé structures. For aromatic hydrocarbon rings it is immaterial which Kekulé structure is used because “splitting” the double bonds gives the same result in all cases; for instance, for phenyl the result can be represented as (12a) where “(6)” denotes the atomic number of the duplicate representations of carbon.



For aromatic hetero rings, each duplicate is given an atomic number that is the mean of what it would have if the double bond were located at each of the possible positions. A complex case is illustrated in (13). Here C-1 is doubly bonded to one or other of the nitrogen atoms (atomic number 7) and never to carbon, so its added duplicate has atomic number 7; C-3 is doubly bonded either to C-4 (atomic number 6) or to N-2 (atomic number 7), so its added duplicate has atomic number $6\frac{1}{2}$; so has that of C-8; but C-4a may be doubly bonded to C-4, C-5, or N-9, so its added duplicate has atomic number 6.33.

One last point about the chiral centre may be added here. Except for hydrogen, ligancy, if not already four, is made up to four by adding “phantom atoms” which have atomic number zero and are thus always last in order of preference. This has various uses but perhaps the most interesting is where nitrogen occurs in a rigid skeleton, as for example in α -isosparteine (14); here the phantom atom can be placed where the nitrogen lone pair of electrons is; then N-1 appears as shown alongside the formula, and the chirality (*R*) is the consequence; the same applies to N-16. Phantom atoms are similarly used when assigning chirality symbols to chiral sulfoxides (see example to Rule E-5.9).



(14) (1*R*, 6*R*, 7*S*, 9*S*, 11*R*, 16*R*)-Sparteine

Symbolism

In names of compounds, the *R* and *S* symbols, together with their locants, are placed in parentheses, normally in front of the name, as shown for morphine (10) and sparteine (14); but this may be varied in indexes or in languages other than English. Positions within names are required, however, when more than a single series of numerals is used, as for esters and amines. When relative stereochemistry is more

important than absolute stereochemistry, as for steroids or carbohydrates, a local system of stereochemical designation may be more useful and sequence-rule symbols need then be used only for any situations where the local system is insufficient.

Racemates containing a single centre are labelled (*RS*). If there is more than one centre the first is labelled (*RS*) and the others are (*RS*) or (*SR*) according to whether they are *R* or *S* when the first is *R*. For instance, the 2,4-pentanediols $\text{CH}_3\text{—CH(OH)—CH}_2\text{—CH(OH)—CH}_3$ are differentiated as:

one chiral form (*2R,4R*)—
 other chiral form (*2S,4S*)—
meso-compound (*2R,4S*)—
 racemic compound (*2RS,4RS*)—

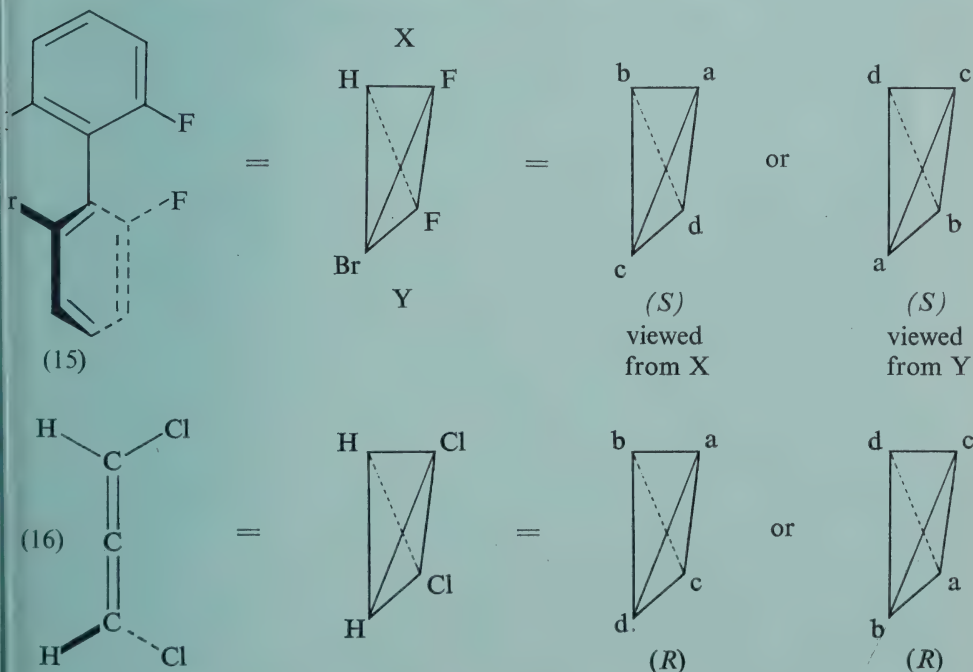
Finally the principles by which some of the least rare of other situations are treated will be very briefly summarized.

Pseudoasymmetric atoms

A sub-rule decrees that *R* groups have preference over *S* groups and this permits pseudo-asymmetric atoms, as in $\text{abC(c-}R\text{)(c-S)}$ to be treated in the same way as chiral centres; but as such a molecule is achiral (not optically active) it is given the lower-case symbol *r* or *s*.

Chiral axis

The structure is regarded as an elongated tetrahedron and viewed along the axis—it is immaterial from which end it is viewed; the nearer pair of ligands receives the first two positions in the order of preference, as shown in (15) and (16).



Chiral plane

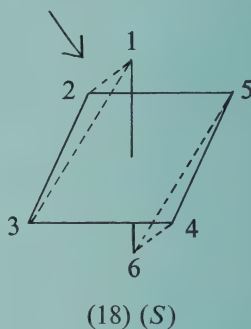
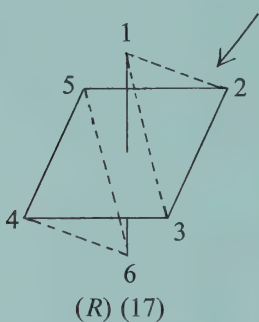
The sequence-rule-preferred atom directly attached to the plane is chosen as "pilot atom". In compound (3) (page 72) this is the C of the left-hand CH_2 group. Now this is attached to the left-hand oxygen atom in the plane. The sequence-rule-preferred path from this oxygen atom is then explored in the plane until a rotation is traced which is clockwise (*R*) or anticlockwise (*S*) when viewed from the pilot atom. In (3) this path is $\text{O} \rightarrow \text{C} \rightarrow \text{C}(\text{Br})$ and it is clockwise (*R*).

Other sub-rules

Other sub-rules cater for new chirality created by isotopic labelling (higher mass number preferred to lower) and for steric differences in the ligands. Isotopic labelling rarely changes symbols allotted to other centres.

Octahedral structures

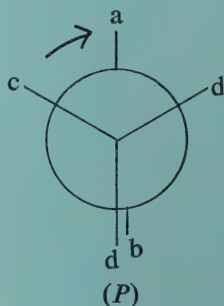
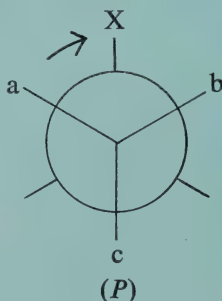
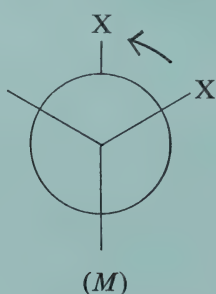
Extensions of the sequence rule enable ligands arranged octahedrally to be placed in an order of preference, including polydentate ligands, so that a chiral structure can then always be represented as one of the enantiomeric forms (17) and (18). The face



1—2—3 is observed from the side remote from the face 4—5—6 (as marked by arrows), and the path 1→2→3 is observed; in (17) this path is clockwise (*R*), and in (18) it is anticlockwise (*S*).

Conformations

The torsion angle between selected bonds from two singly bonded atoms is considered. The selected bond from each of these two atoms is that to a unique ligand, or otherwise to the ligand preferred by the sequence rule. The smaller rotation needed to make the front ligand eclipsed with the rear one is noted (this is the rotatory characteristic of a helix); if this rotation is right-handed it leads to a symbol *P* (plus); if left-handed to *M* (minus). Examples are:



Details and complications

For details and complicating factors the original papers should be consulted. They include treatment of compounds with high symmetry or containing repeating units (*e.g.*, cyclitols), also π -bonding (metallocenes, etc.), mesomeric compounds and mesomeric radicals, and helical and other secondary structures.

Some common groups in order of sequence-rule preference

Note: ANY alteration to structure, or substitution, etc., may alter the order of preference.

A. Alphabetical order: higher number denotes greater preference

64 Acetoxy	28 3,5-Dinitrophenyl	70 Methylthio
36 Acetyl	59 Ethoxy	11 Neopentyl
48 Acetylamino	40 Ethoxycarbonyl	56 Nitro
21 Acetylenyl	3 Ethyl	27 <i>m</i> -Nitrophenyl
10 Allyl	46 Ethylamino	33 <i>o</i> -Nitrophenyl
43 Amino	68 Fluoro	24 <i>p</i> -Nitrophenyl
44 Ammonio $^+H_3N-$	35 Formyl	55 Nitroso
37 Benzoyl	63 Formyloxy	6 <i>n</i> -Pentyl
49 Benzoylamino	62 Glycosyloxy	61 Phenoxy
65 Benzoyloxy	7 <i>n</i> -Hexyl	42 Phenoxycarbonyl
50 Benzyloxycarbonylamino	1 Hydrogen	22 Phenyl
13 Benzyl	57 Hydroxy	47 Phenylamino
60 Benzyloxy	76 Iodo	54 Phenylazo
41 Benzyloxycarbonyl	9 Isobutyl	18 Propenyl
75 Bromo	8 Isopentyl	4 <i>n</i> -Propyl
42 <i>tert</i> -Butoxycarbonyl	20 Isopropenyl	29 1-Propynyl
5 <i>n</i> -Butyl	14 Isopropyl	12 2-Propynyl
16 <i>sec</i> -Butyl	69 Mercapto	73 Sulfo
19 <i>tert</i> -Butyl	58 Methoxy	25 <i>m</i> -Tolyl
38 Carboxyl	39 Methoxycarbonyl	30 <i>o</i> -Tolyl
74 Chloro	2 Methyl	23 <i>p</i> -Tolyl
17 Cyclohexyl	45 Methylamino	53 Trimethylammonio
52 Diethylamino	71 Methylsulfinyl	32 Trityl
51 Dimethylamino	66 Methylsulfinyloxy	15 Vinyl
34 2,4-Dinitrophenyl	72 Methylsulfonyl	31 2,6-Xylyl
	67 Methylsulfonyloxy	26 3,5-Xylyl

B. Increasing order of sequence-rule preference

1 Hydrogen	28 3,5-Dinitrophenyl	55 Nitroso
2 Methyl	29 1-Propynyl	56 Nitro
3 Ethyl	30 <i>o</i> -Tolyl	57 Hydroxy
4 <i>n</i> -Propyl	31 2,6-Xylyl	58 Methoxy
5 <i>n</i> -Butyl	32 Trityl	59 Ethoxy
6 <i>n</i> -Pentyl	33 <i>o</i> -Nitrophenyl	60 Benzyloxy
7 <i>n</i> -Hexyl	34 2,4-Dinitrophenyl	61 Phenoxy
8 Isopentyl	35 Formyl	62 Glycosyloxy
9 Isobutyl	36 Acetyl	63 Formyloxy
10 Allyl	37 Benzoyl	64 Acetoxy
11 Neopentyl	38 Carboxyl	65 Benzoyloxy
12 2-Propynyl	39 Methoxycarbonyl \diamond	66 Methylsulfinyloxy
13 Benzyl	40 Ethoxycarbonyl \diamond	67 Methylsulfonyloxy
14 Isopropyl	41 Benzyloxycarbonyl \diamond	68 Fluoro
15 Vinyl	42 <i>tert</i> -Butoxycarbonyl \diamond	69 Mercapto HS—
16 <i>sec</i> -Butyl	43 Amino	70 Methylthio CH_3S-
17 Cyclohexyl	44 Ammonio $^+H_3N-$	71 Methylsulfinyl
18 1-Propenyl	45 Methylamino	72 Methylsulfonyl
19 <i>tert</i> -Butyl	46 Ethylamino	73 Sulfo HO_3S-
20 Isopropenyl	47 Phenylamino	74 Chloro
21 Acetylenyl	48 Acetylamino	75 Bromo
22 Phenyl	49 Benzoylamino	76 Iodo
23 <i>p</i> -Tolyl	50 Benzyloxycarbonylamino	
24 <i>p</i> -Nitrophenyl	51 Dimethylamino	
25 <i>m</i> -Tolyl	52 Diethylamino	
26 3,5-Xylyl	53 Trimethylammonio	
27 <i>m</i> -Nitrophenyl	54 Phenylazo	

\diamond These groups are $RO-\overset{\overset{O}{\parallel}}{C}-$.

IUPAC-SPONSORED MEETINGS

1969

June 17-20	Colloque Weyl-II: The nature of metal-ammonia solutions (Prof. J.J. LAGOWSKI, Department of Chemistry, University of Texas at Austin, Austin, Texas 78712, USA)	Ithaca (USA)
June 30- July 8	XXVth International Conference of Pure and Applied Chemistry (Executive Secretary, IUPAC Secretariat, Bank Court Chambers, 2/3 Pound Way, Cowley Centre, Oxford OX4 3YF, UK)	Cortina d'Ampezzo (Italy)
July 9-10	Symposium on the Chemical Aspects of Air Pollution (Dr V. CANTUTI, Laboratorio sull'Inquinamento atmosferico, c/o Istituto di Chimica analitica, Università di Roma, 00185 Roma, Italy)	Cortina d'Ampezzo (Italy)
July 14-18	International Atomic Absorption Spectroscopy Conference (IAAS Conference Secretary, Society for Analytical Chemistry, 9/10 Savile Row, London W 1, UK)	Sheffield (UK)
July 14-18	International Symposium on the Chemical Control of the Human Environment (IUPAC Symposium Secretary, c/o SA Council for Scientific and Industrial Research, PO Box 395, Pretoria, Republic of South Africa)	Johannesburg (South Africa)
July 16-18	Symposium on Surface Area Determination (Dr R. H. OTTEWILL, Secretary, Symposium on Surface Area Determination, School of Chemistry, University of Bristol, Cantock's Close, Bristol BS8 1TS, UK)	Bristol (UK)
July 21-25	International Symposium on Analytical Chemistry (Mr D. M. PEAKE, Secretary, International Symposium on Analytical Chemistry, 61 Lodge Road, Walsall, Staffordshire, UK)	Birmingham (UK)
July 27- August 1	IVth International Symposium on Organometallic Chemistry (Dr E. W. ABEL, Secretary, IVth International Conference on Organometallic Chemistry, School of Chemistry, University of Bristol, Cantock's Close, Bristol BS8 1TS, UK)	Bristol (UK)
August 20-27	XXIInd International Congress of Pure and Applied Chemistry and XIIth International Conference on Co-ordination Chemistry (Organizing Committee, XXIInd IUPAC/XIIth ICC, Box 2249U, GPO, Melbourne, Australia 3001)	Sydney (Australia)
August 25-30	International Symposium on Macromolecular Chemistry: Kinetics and mechanism of polyreactions (Secretariat of the Symposium on Macromolecular Chemistry, Budapest II, Pustzaszeri út 59-67, Hungary)	Budapest (Hungary)
September 1-4	IVth Microsymposium: Rheology of polymer solids and concentrated solutions (Institute of Macromolecular Chemistry, Czechoslovak Academy of Sciences, Prague 6 - Petřiny, Czechoslovakia)	Prague (Czechoslovakia)
September 1-3	Vth Microsymposium: Cyclopolymers and cyclopolymerization (Institute of Macromolecular Chemistry, Czechoslovak Academy of Sciences, Prague 6 - Petřiny, Czechoslovakia)	Prague (Czechoslovakia)
September 8-11	VIth Microsymposium: Light scattering in polymer science (Institute of Macromolecular Chemistry, Czechoslovak Academy of Sciences, Prague 6 - Petřiny, Czechoslovakia)	Prague (Czechoslovakia)
September 8-12	International Symposium on Conformational Analysis (Executive Secretary, International Symposium on Conformational Analysis, 49, square Marie-Louise, Bruxelles 4, Belgium)	Brussels (Belgium)
October 16-19	International Symposium on University Chemical Education (Prof. G. ILLUMINATI, Istituto Chimico, Università di Roma, 00185 Roma, Italy)	Frascati (Italy)

1970

April 1-4	International Conference on Thermodynamics (Dr W. J. HORNIX, Secretary of Organizing Committee, Department of Applied Mathematics and Mathematical Physics, University College of South Wales, Cardiff CFI 3NR, UK)	Cardiff (UK)
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June 22-27	VIIth International Symposium on the Chemistry of Natural Products (Prof. S.N.ANANCHENKO, General Secretary, VIIth International Symposium on the Chemistry of Natural Products, Institute for Chemistry of Natural Products, Academy of Sciences of USSR, ul. Vavilova 18, Moscow 312, USSR)	Riga (USSR)
July 6-11	Symposium on Non-aqueous Electrochemistry: Organic and Inorganic Solvents including Fused Salts (Mme J.BADOZ-LAMBLING, Laboratoire de Chimie analytique, Ecole supérieure de Physique et de Chimie industrielles, 10, rue Vauquelin, Paris 5 ^e , France)	Paris (France)
July 12-18	IIIrd International Symposium on Photochemistry (Prof. D. BRYCE-SMITH, Department of Chemistry, University of Reading, Whiteknights Park, Reading, Berkshire, UK)	St. Moritz (Switzerland)
August 25-30	International Symposium on the Chemistry of Nonbenzenoid Aromatic Compounds (Prof. S.Irô, General Secretary, International Symposium on the Chemistry of Nonbenzenoid Aromatic Compounds, Department of Chemistry, Tohoku University, Sendai, Japan)	Sendai (Japan)
September 7-11	VIth International Symposium on Microtechniques (Sekretariat des VI. Internationalen Symposiums für Mikrochemie, c/o INTERCONGRESS, Stadiongasse 6-8, A-1010 Wien, Austria)	Graz (Austria)
September 11-18	XIIIth International Conference on Co-ordination Chemistry (Dr K.BUKIETYŃSKA, Secretary, XIIIth International Conference on Co-ordination Chemistry, Uniwersytet Wrocławski, Katedra Chemii Nieorganicznej, Wrocław, Poland)	Zakopane/ Cracow (Poland)
September 14-17	Symposium on Cycloaddition (Prof. R. HUISGEN, Institut für Organische Chemie der Universität München, Karlstrasse 23, 8000 München 2, Germany)	Munich (Germany)
September 20-24	Conference on Analytical Chemistry (Hungarian Chemical Society, Szabadság tér 17, Budapest V, Hungary)	Budapest (Hungary)
September 8-11	Symposium on Chemistry of Pesticides under Metabolic and Environmental Conditions (Prof. F. KORTE, Institut für ökologische Chemie der Gesellschaft für Strahlenforschung mbH, München, 5201 Schloss Birlinghoven, Germany)	Bonn (Germany)
1971		
February	Symposium on Chemistry of Terminal Pesticide Residues (Dr C. RESNICK, Ministry of Agriculture, PO Box 15030, Jaffa, Israel)	Tel Aviv
July 19-24	XXVIth International Conference of Pure and Applied Chemistry (Executive Secretary, IUPAC Secretariat, Bank Court Chambers, 2/3 Pound Way, Cowley Centre, Oxford OX4 3YF, UK)	Washington, DC (USA)
July 25-31	XXIIIrd International Congress of Pure and Applied Chemistry (Prof. P.D.BARTLETT, Chairman of Programme Committee, XXIIIrd International Congress of Pure and Applied Chemistry, Department of Chemistry, Harvard University, 12 Oxford Street, Cambridge, Mass. 02138, USA)	Boston (USA)
Summer	IIIrd International Conference on Crystal Growth (Dr B. MUTAF-TSHIEV, Laboratoire de Minéralogie-Cristallographie, Université d'Aix-Marseille, Marseille, France)	Marseille (France)
1972		
April 3-7	International Congress on Analytical Chemistry (Prof. T.FUJINAGA, Faculty of Sciences, University of Kyoto, Kyoto, Japan)	Kyoto (Japan)
August	Vth International Congress on Catalysis (Prof. R.L. BURWELL, Jr, Department of Chemistry, Northwestern University, Evanston, Illinois 60201, USA)	(USA)

CALENDAR OF NON-IUPAC MEETINGS

1969

June 16-20	IXth Conference on Carbon (Dr A.I. MEDALIA, c/o Cabot Corporation, Concord Road, Billerica, Mass. 01821, USA)	Boston (USA)
June 23-27	LXIVth Annual Meeting of Association of Cellulose and Paper Analytical Chemists and Engineers (Verein der Zellstoff- und Papier-Chemiker und -Ingenieure, Rheinstrasse 51, 61 Darmstadt, Germany)	Baden-Baden (Germany)
June 23-July 7	International Summer School "Chemistry of Solid/Liquid Interfaces" (Prof. B. TEZAK, Institute "Rudjer Boskovic", POB 171, Zagreb, Yugoslavia)	Herceg Novi (Yugoslavia)
July 1-3	International Symposium on Chemical Effects of Nuclear Transformations (Dr J. F. GIBSON, Scientific Affairs Officer, The Chemical Society, Burlington House, London W1V 0BN, UK)	Cambridge (UK)
July 7-11	International Colloquium on Structure and Properties of Solid Surfaces (Prof. J. BÉNARD, Ecole Nationale supérieure de Chimie, 11, rue Pierre-Curie, Paris-5 ^e , France)	Paris (France)
July 7-11	IIInd International Congress of Heterocyclic Chemistry (Secrétariat du Deuxième Congrès International de Chimie hétérocyclique, Service de M. le Professeur JACQUIER, Faculté des Sciences, Place Eugène Bataillon, 34-Montpellier, France)	Montpellier (France)
July 8-10	International Symposium on Isotope Effects (Dr J.F. GIBSON, Scientific Affairs Officer, The Chemical Society, Burlington House, London W1V 0BN, UK)	York (UK)
July 9-12	Symposium on Gas Kinetics (Dr T. BERCES, c/o Institute of General and Physical Chemistry, University of Szeged, POB 105, Szeged, Hungary)	Szeged (Hungary)
July 14-18	IVth International Congress for Pharmacology (Dr F.J. BOVE, Secretary of Organizing Committee, IVth International Congress for Pharmacology, Postfach 30, 4000 Basle 4, Switzerland)	Basle (Switzerland)
July 15-16	International Symposium on Enamine Chemistry (Dr P. W. HICKMOTT, Department of Chemistry, University of Salford, Salford M5 4WT, UK)	Salford (UK)
July 15-19	International Symposium on Nuclear Magnetic Resonance (Dr J.F. GIBSON, Scientific Affairs Officer, The Chemical Society, Burlington House, London W1V 0BN, UK)	Birmingham (UK)
July 16-18	International Conference on Ion Exchange in the Process Industries (Society of Chemical Industry, 14 Belgrave Square, London SW1, UK)	London (UK)
July 20-21	Vth International Symposium on Fluorine Chemistry (Symposium Committee, Vavilova St. 28, Moscow V-312, USSR)	Moscow (USSR)
July 22-24	International Symposium on Synthetic Methods and Rearrangements in Alicyclic Chemistry (Dr J.F. GIBSON, Scientific Affairs Officer, The Chemical Society, Burlington House, London W1V 0BN, UK)	Oxford (UK)
July 28-August 1	Symposium on the Physics and Chemistry of Fission (International Atomic Energy Agency, Kärntner Ring 11, Vienna 1, Austria)	Vienna (Austria)
August 10-15	VIth International Congress of Chemotherapy (Dr W.P. BOGER, POB 265, Princeton, N.J. 08549, USA)	Tokyo (Japan)
August 11-14	International Symposium on Electron and Nuclear Magnetic Resonance (Executive Secretary, Australian Academy of Science, Gordon Street, Canberra City, ACT, Australia 2601)	Clayton (Australia)

August 12-15	IIIrd International Photoconductivity Conference (G.S.PICUS, Conference Secretary, IIIrd International Photoconductivity Conference, Hughes Research Laboratories, 3011 Malibu Canyon Road, Malibu, Calif. 90265, USA)	Palo Alto (USA)
August 13-21	VIIIth General Assembly and International Congress of International Union of Crystallography (Mrs N.FIESS, Executive Secretary, International Union of Crystallography Congress Headquarters, Room 254, ES & S, State University of New York at Stony Brook, Stony Brook, N.Y. 11790, USA)	New York (USA)
August 31- September 3	International Wood Chemistry Symposium (Profs K.V.SARKANEN and J.L.McCARTHY, Benson Hall, University of Washington, Seattle, Washington 98105, USA)	Seattle (USA)
August 31- September 4	Ist International Conference on Calorimetry and Thermodynamics (Dr H.KHAIAN, Secretary of Organizing Committee, Ist International Conference on Calorimetry and Thermodynamics, Institute of Physical Chemistry, Polish Academy of Sciences, PO Box 49, Warsaw 42, Poland)	Warsaw (Poland)
September 3-5	XVth Canadian High Polymer Forum (Dr R.St.JOHN MANLEY, Secretary-Treasurer, XVth Canadian High Polymer Forum, c/o Pulp and Paper Research Institute, McGill University, Montreal, Que., Canada)	Kingston (Canada)
September 3-6	Congress on Chemistry in Agriculture (Organization Committee Secretariat, POB 197, Bratislava 1, Czechoslovakia)	Bratislava (Czechoslovakia)
September 4-6	Lth Polish Chemical Society National Congress (Ul. Freta 16, Warsaw, Poland)	Krakow (Poland)
September 7-12	XIth Biennial Conference of International Union of Leather Chemists Societies (3 William Street, Hurstead, Rochdale, Lancashire, UK)	London (UK)
September 8-10	International Symposium on Distillation (Institution of Chemical Engineers, 16 Belgrave Square, London SW1, UK)	Brighton (UK)
September 8-12	International Conference on Mass Spectroscopy (Mr K. OGOTA, c/o Dept. of Physics, Faculty of Science, Osaka University, Toyonaka-Shi, Osaka, Japan)	Kyoto (Japan)
September 8-13	VIIth International Congress of Clinical Chemistry (Dr M.ROTH, Secretary, VIIth International Congress of Clinical Chemistry, Palais des Expositions, 16, quai de l'Ecole de Médecine, CH-1211 Genève 4, Switzerland)	Geneva (Switzerland)
September 8-13	International Symposium on Atmospheric Chemistry and Radioactivity (Dr E.A. MARTELL, Secretary, Commission on Atmospheric Chemistry and Radioactivity, International Association of Meteorology and Atomospheric Physics, c/o National Centre for Atomospheric Research, POB 1470, Boulder, Colo. 8302, USA)	Heidelberg (Germany)
September 9-12	XXXIXth International Congress of Industrial Chemistry (General Secretariat, Halaskargazi Caddesi No. 53 KAT 8, Istanbul, Turkey)	Istanbul (Turkey)
September 10-14	IInd Symposium on Ion-Exchange (Hungarian Chemical Society, Szabadsag ter 17, Budapest, Hungary)	Balatonszeplak (Hungary)
September 13-19	International Association of Volcanology and Chemistry of the Earth's Interior Symposium (Prof. P. EVRARD, c/o Institut de Géologie, 45, av. des Tilleuls, Liège, Belgium)	Edinburgh (UK)
September 14-20	XXth Meeting of International Committee of Electrochemical Thermodynamics and Kinetics (Dr H. TANNENBERGER, Secretary General CITCE, c/o Institut Battelle, 7, route de Drize, CH-1227 Carouge-Genève, Switzerland)	Strasbourg (France)

September 15-20	International Congress of Chemical Engineering, Chemical Equipment and Automation (III CHISA 1969, Czechoslovak Scientific and Technical Society, PO Box 857, Prague 1, Czechoslovakia)	Marianske Lazne (Czechoslovakia)
September 15-20	General Assembly of The German Chemical Society (GDCh-Geschäftsstelle, 6000 Frankfurt (M), Postfach 119075, Germany)	Hamburg (Germany)
September 22-25	Symposium on Co-ordination Chemistry of Transition Elements (Chemische Gesellschaft in der DDR, Clara-Zetkin-Strasse 105, 108 Berlin, Germany)	Jena (Germany)
September 22-23	International Conference on the Use of Cyclotrons in Chemistry, Metallurgy and Biology (F. K. PYNE, Conference Secretary, International Conference on the Use of Cyclotrons in Chemistry, Metallurgy and Biology, Atomic Energy Research Establishment, Harwell, Didcot, Berkshire, UK)	Oxford (UK)
October 16-17	Meeting of Federation of Belgian Chemical Industries (M. J. M. DAQUETTE, Directeur, Federation of Belgian Chemical Industries, 49, square Marie-Louise, Bruxelles 4, Belgium)	Brussels (Belgium)
November or December	Symposium on Chemicals and Oils from Coal (Dr N. G. BASAK, Deputy Director, Central Fuel Research Institute, PO FRI, Dhanbad, Bihar, India)	Dhanbad (India)

LIST OF ABBREVIATIONS

AOAC	Association of Official Agricultural Chemists
CBN	Commission on Biochemical Nomenclature
CEBJ	Commission of Editors of Biochemical Journals
CEE	Communauté Economique Européenne
CIG	Comité International de Géophysique
CIPM	Comité International de Poids et Mesures
CITCE	Comité International de Thermodynamique et Cinétique Electrochimique
CNRS	Centre national de la Recherche scientifique
COMECON	Council for Mutual Economic Assistance
COSPAR	Committee on Space Research
CSF	Compagnie Télégraphie Sans Fil
CSIRO	Commonwealth Scientific and Industrial Research Organization
DECHEMA	Deutsche Gesellschaft für chemisches Apparatewesen eV
EEC	European Economic Community
EMPA	Eidgenössische Materialprüfungs-Anstalt
EPPO	European and Mediterranean Plant Protection Organization
ETH	Eidgenössische Technische Hochschule (Zürich)
EUCEPA	European Committee on Cellulose and Paper
EUROTOX	Comité européen permanent pour la Protection des populations contre les risques de toxicité à long terme
FAGS	Fédération of Astronomical and Geophysical Services
FAO	Food and Agriculture Organization
GEFAP	Groupeement européen des Associations nationales de Fabricants de Pesticides
IAEA	International Atomic Energy Agency
IAMS	International Association of Microbiological Societies
IAPT	International Association for Plant Taxonomy
IASH	International Association of Scientific Hydrology
IAU	International Astronomical Union
IBP	International Biological Programme
ICCA	International Commission for Cellulose Analysis
ICSU	International Council of Scientific Unions
ICUMSA	International Committee for the Unification of Methods of Sugar Analysis
IGU	International Geographical Union
IMU	International Mathematical Union
ISO	International Organization for Standardization
ITU	International Telecommunication Union
IUB	International Union of Biochemistry
IUBS	International Union of Biological Sciences
IUCr	International Union of Crystallography
IUGG	International Union of Geodesy and Geophysics
IUGS	International Union of Geological Sciences
IUNS	International Union of Nutritional Sciences
IUPAC	International Union of Pure and Applied Chemistry
IUPAP	International Union of Pure and Applied Physics

JCAM	Joint Commission on Atomic Masses
JCAR	Joint Commission on Applied Radioactivity
MIT	Massachusetts Institute of Technology
NAS	National Academy of Sciences
NATO	North Atlantic Treaty Organization
NBS	National Bureau of Standards
NRC	National Research Council
OECD	Organisation de Coopération et de Développement économiques
OEPP	Organisation européenne de Protection des Plantes
OMS	Organisation Mondiale de la Santé
SCAR	Scientific Committee on Antarctic Research
SCOR	Scientific Committee on Oceanic Research
UICC	Union internationale contre le Cancer
UNESCO	United Nations Educational Scientific and Cultural Organization
WHO	World Health Organization
WMO	World Meteorological Organization

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